

Supplementary data for the article:

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Supporting Information

Unraveling the Role of a Flexible Tetradentate Ligand in the Aerobic Oxidative Carbon-Carbon Bond Formation with Palladium Complexes: A Computational Mechanistic Study

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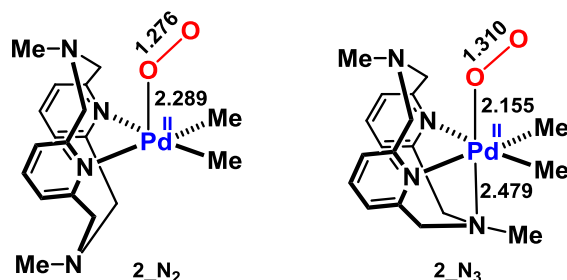
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Relative energy of (^{Me}L)Pd^{II} complex with O₂ adducts

To better evaluate the relative energy level of spin states, we had applied several DFT functional to calculate the single point energy of singlet structure with considerations of possible extra N coordinated in the complex Pd^{II}N₃-O₂ (Table 1). The energy deviation of any selected functional is within 4.0 kcal/mol for each complex. All the tested functional shown triplet spin states are most stable in contrast to singlet state that is unstable. And the similar trend was also found in Pd^{II}N₃-O₂ complex that involve an additional N-ligand coordinated to Pd^{II} from the axial direction. Comparing the energies of N₂ and N₃ coordinated systems of (^{Me}L)Pd-O₂, Triplet and Open-shell singlet species favor to form N₂ complex about 7.0 and 5.0 kcal/mol, respectively, while singlet species favor N₃ coordination 2.7 kcal/mol at B3LYP-D3 level.

TableS1. Relative energies of Pd^{II}N₂-O₂ and Pd^{II}N₃-O₂ complex based on singlet structures



	Pd ^{II} _N ₂ /Pd ^{II} _N ₃ (kcal/mol)					
functional	B3LYP	B3LYP-D3	TPSS	TPSSh	M06	M06L
Singlet	0.0/-1.6	0.0/-2.7	0.0/-4.6	0.0/-3.5	0.0/-1.5	0.0/-4.0
O-Singlet ^{a,b}	-11.3/-5.7	-11.3/-6.8	-9.4/-4.6	-11.5/-6.3	-7.7/-6.3	-7.8/-3.0
Triplet ^b	-17.3/-9.2	-17.3/-10.3	-13.8/-7.0	-16.3/-9.2	-17.7/-9.2	-16.8/-8.8

a. Open shell singlet, b. relative single point energy comparing to singlet state of B3LYP method.

Coordination of (^{Me}L)Pd^{II} complex with O₂ adducts

Possible coordination of (^{Me}L)Pd(II) and O₂ were tried to further describe the stability of singlet and triplet spin states shown in Figure S1. In the single O coordination, there are only slightly influences to the singlet adduct energies of (^{Me}L)Pd(II) and O₂, when we localize stable structure in each 90° shown in Figure S1A. And the triplet adducts still favor dissociation of O₂ in all the tested O₂ orientation. The double O coordination in Figure S1B was unfavorable, because it trend to transform to single O coordination whatever spin state you used. Removing one ligand binding of ligand (^{Me}L), we were able to optimize the structures of singlet and triplet state with high energy, although two forms of O coordination can be located on the basis of singlet state (Figure S1C). All the calculations indicate that 2_ N2 is hard to form a stable triplet complex and triplet O₂ prefers to dissociate from Pd^{II} center.

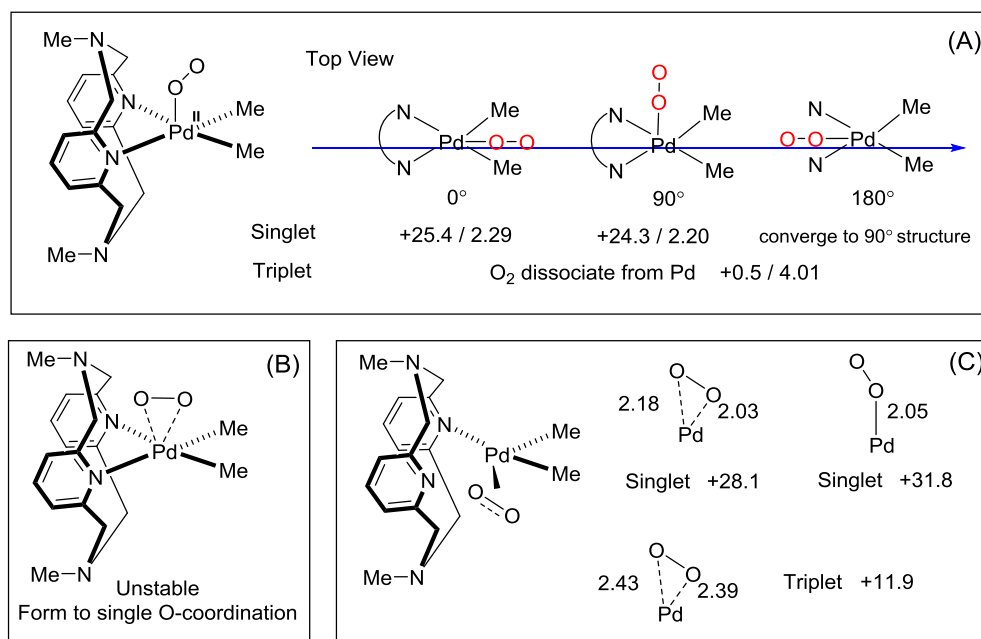


Figure S1. Possible coordination of (^{Me}L)Pd^{II} and O₂. (A) Single O-coordinations to Pd center depending on O₂ orientations. E(kcal/mol) / Pd-O distances (Å); (B) O-O coordination to Pd center; (C) The coordination of (^{Me}L)Pd^{II} and O₂, while ligand (^{Me}L) contribute only one pyridine arm. E (kcal/mol), Pd-O distances (Å).

Explicit solvent models of (^{Me}L)Pd^{II}-O₂ adducts.

The figure S2 suggest a good trend to form 4_N₃ triplet adducts with increasingly H₂O involved. However, this trend cannot be applied to 4_N₂ triplet adducts that is more favorable to release O₂.

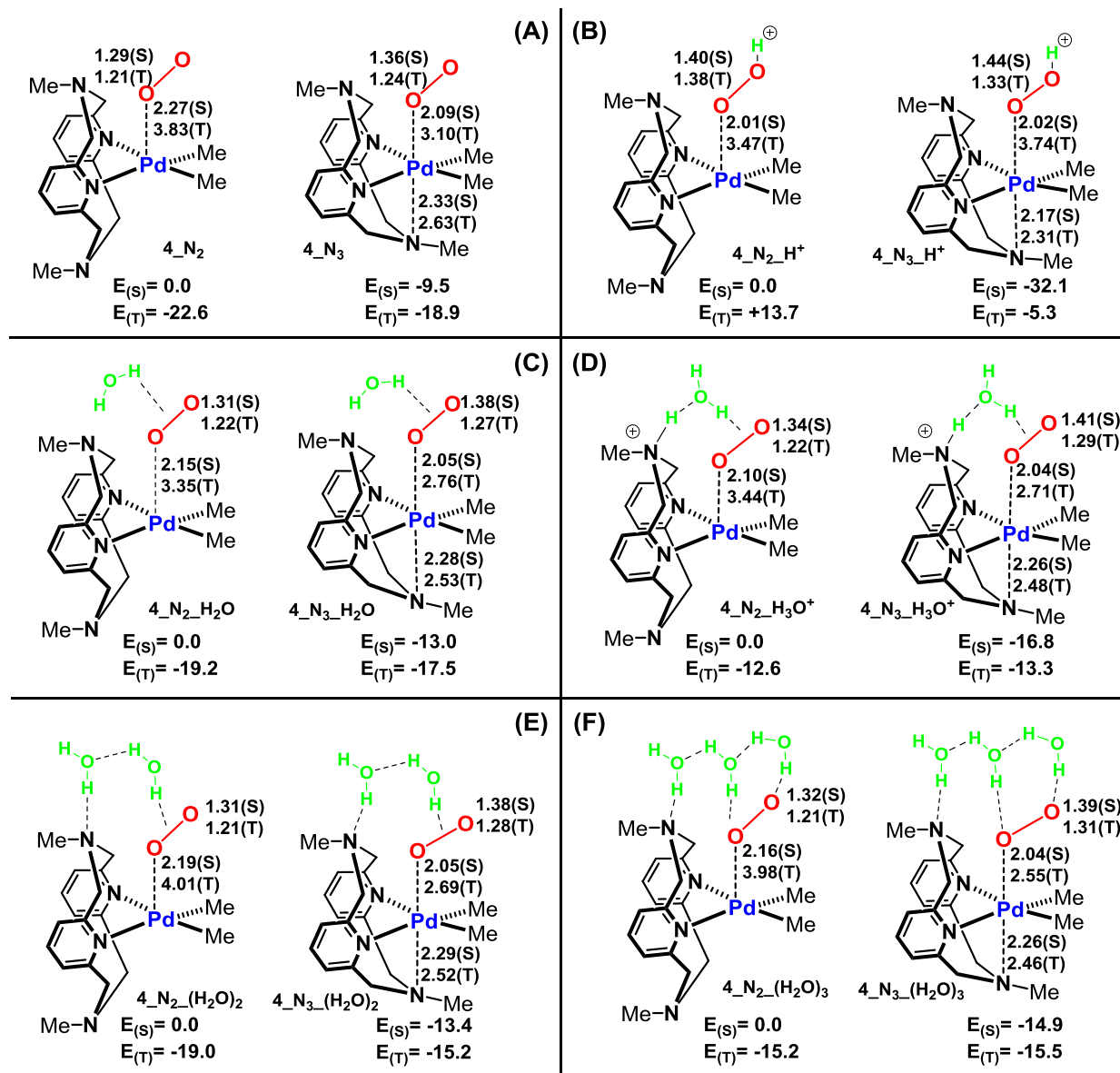


Figure S2. Explicit solvent models of (^{Me}L)Pd^{II}-O₂ adducts. (A) Null; (B) H⁺; (C) H₂O; (D) H₃O⁺; (E) (H₂O)₂; (F) (H₂O)₃. E_S: the relative energies of singlet states, E_T: the relative energies of triplet states. The distances of Pd-O, O-O and Pd-N_{ax} are depicted in the Figure. All units of the energies and distances are shown in kcal/mol and Å, respectively.

Tendency of spin crossover area of $(^{\text{Me}}\text{L})\text{Pd}^{\text{II}}\text{-O}_2$ adducts with effect of H_2O and H^+

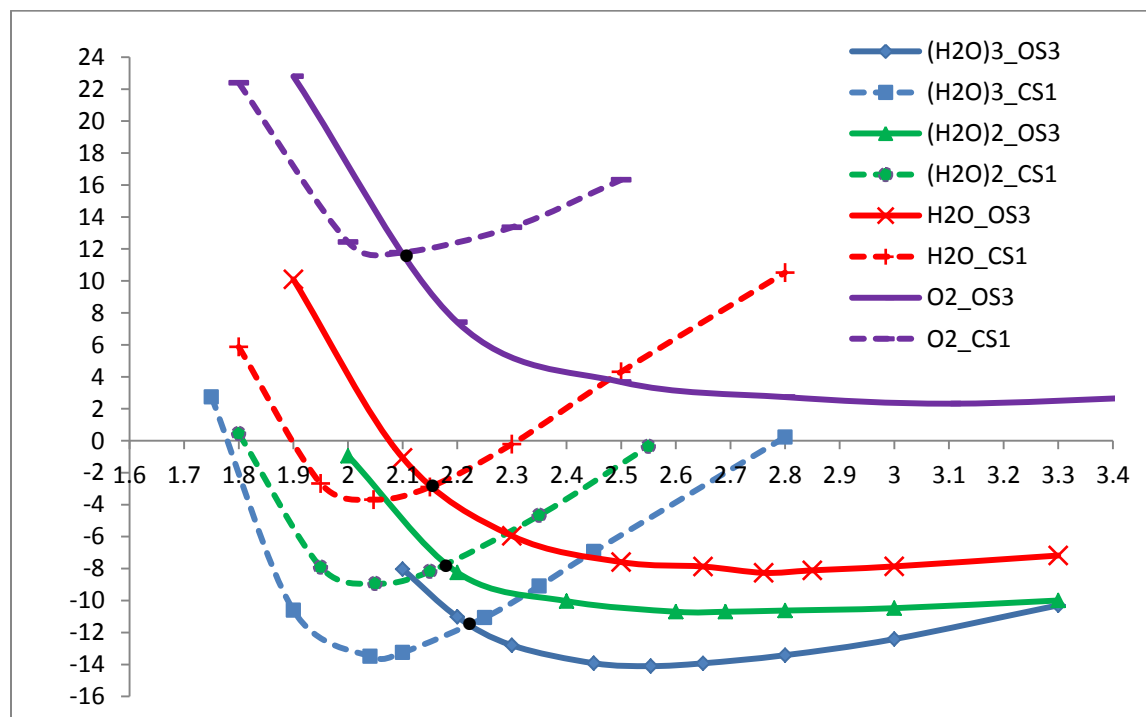


Figure S3. Energy profile for the oxygenation of $(^{\text{Me}}\text{L})\text{Pd}^{\text{II}}\text{Me}_2\text{-N}_3$ involving explicit H_2O , and the area of spin crossover between singlet state and triplet state

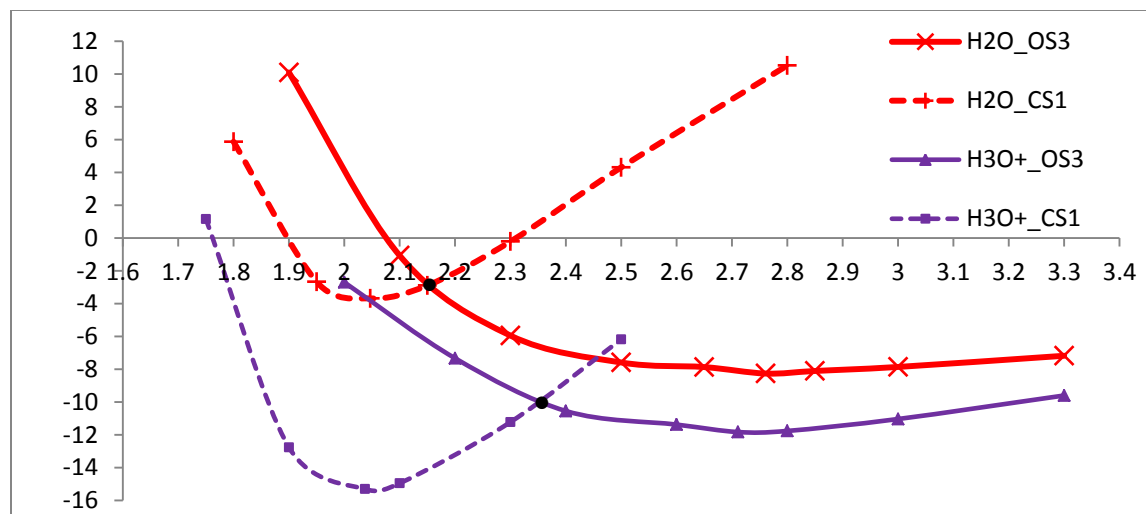


Figure S4. Energy profile for the oxygenation of $(^{\text{Me}}\text{L})\text{Pd}^{\text{II}}\text{Me}_2\text{-N}_3$ involving with H^+ effect, and the area of spin crossover between singlet state and triplet state

Tendency of spin density of triplet ($^{\text{MeL}}$)Pd^{II}-O₂ adducts with effect of H₂O and H⁺

Spin density increasingly move to Pd centre with more H₂O or H⁺ involved.

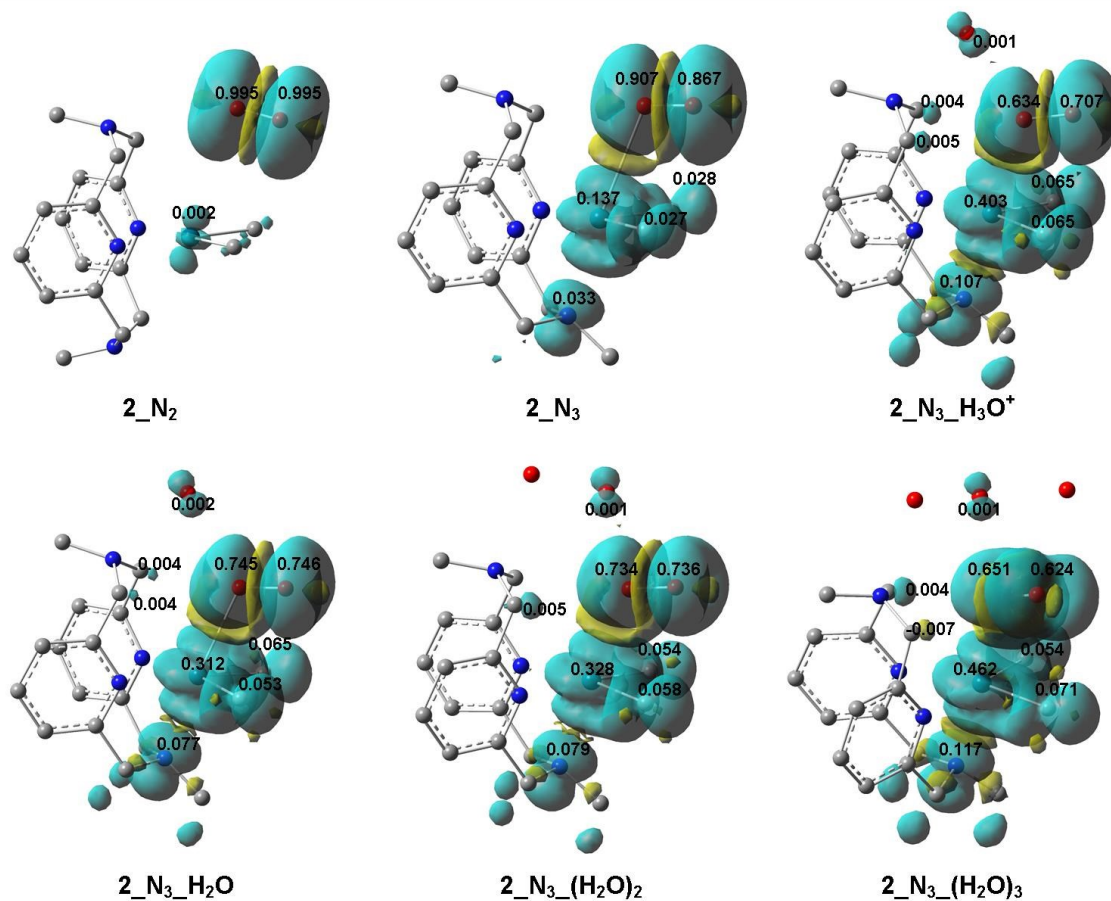


Figure S5. Spin densities of selected triplet states of Figure 3. Isovalue=0.0004. Hydrogen atoms have been removed for clarity.

Frontier orbitals of (MeL)PdII Me₂ complex 1 reacting with triplet O₂.

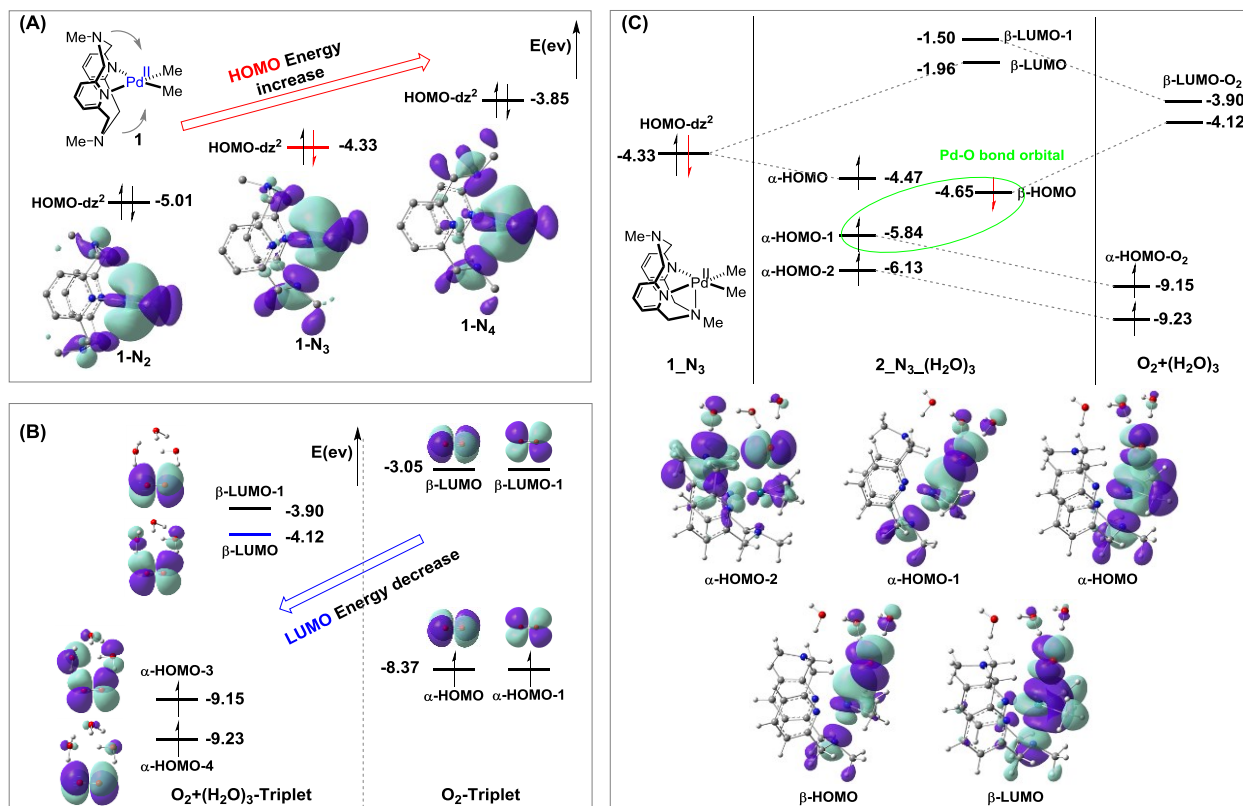


Figure S6. Frontier orbitals of (MeL)PdII Me₂ complex 1 reacting with triplet O₂. (A) Frontier orbitals (HOMOs) of complex 1 with various coordinations; (B) frontier orbitals of triplet O₂ with/without H₂O involved; (C) Molecular diagram for forming the (MeL)PdII Me₂-O₂(H₂O)₃ triplet complex (2_N3).

Figure 1: Energy level diagram and molecular orbital visualizations for the Pd complex. The diagram shows the energy levels (E in eV) for the complex **1_N3** and its fragments **2_N3(MeOH)3** and **O2+(MeOH)3 Triplet**. The HOMO-dz² orbital of **1_N3** is at -4.33 eV. The HOMO of **2_N3(MeOH)3** is at -4.82 eV, which is the Pd-O bond orbital. The LUMO of **2_N3(MeOH)3** is at -1.87 eV. The LUMO of **O2+(MeOH)3 Triplet** is at -4.22 eV. The diagram also shows the energy levels of the fragments **2_N3(MeOH)3** and **O2+(MeOH)3 Triplet**. The energy levels of the fragments are: **2_N3(MeOH)3**: α-HOMO-1 (-5.85 eV), α-HOMO-2 (-6.00 eV), α-HOMO (-4.37 eV), β-HOMO (-4.82 eV), β-LUMO (-1.87 eV), β-LUMO-1 (-1.53 eV). **O2+(MeOH)3 Triplet**: α-HOMO-O2 (-8.62 eV), α-HOMO-3 (-8.77 eV), β-LUMO-O2 (-4.14 eV), β-LUMO (-4.22 eV). The molecular orbital visualizations show the spatial distribution of the orbitals for **1_N3**, **2_N3(MeOH)3**, and **O2+(MeOH)3 Triplet**.

S8

Scheme of Me transfer to form $(^{\text{Me}}\text{L})\text{Pd}^{\text{IV}}\text{Me}_3$

Scheme S1. The plausible electron transfer mechanism of Me transfer steps at B3LYP-D3/6-311++G**/Lanl2TZ level of theory with SMD solvent model correction.

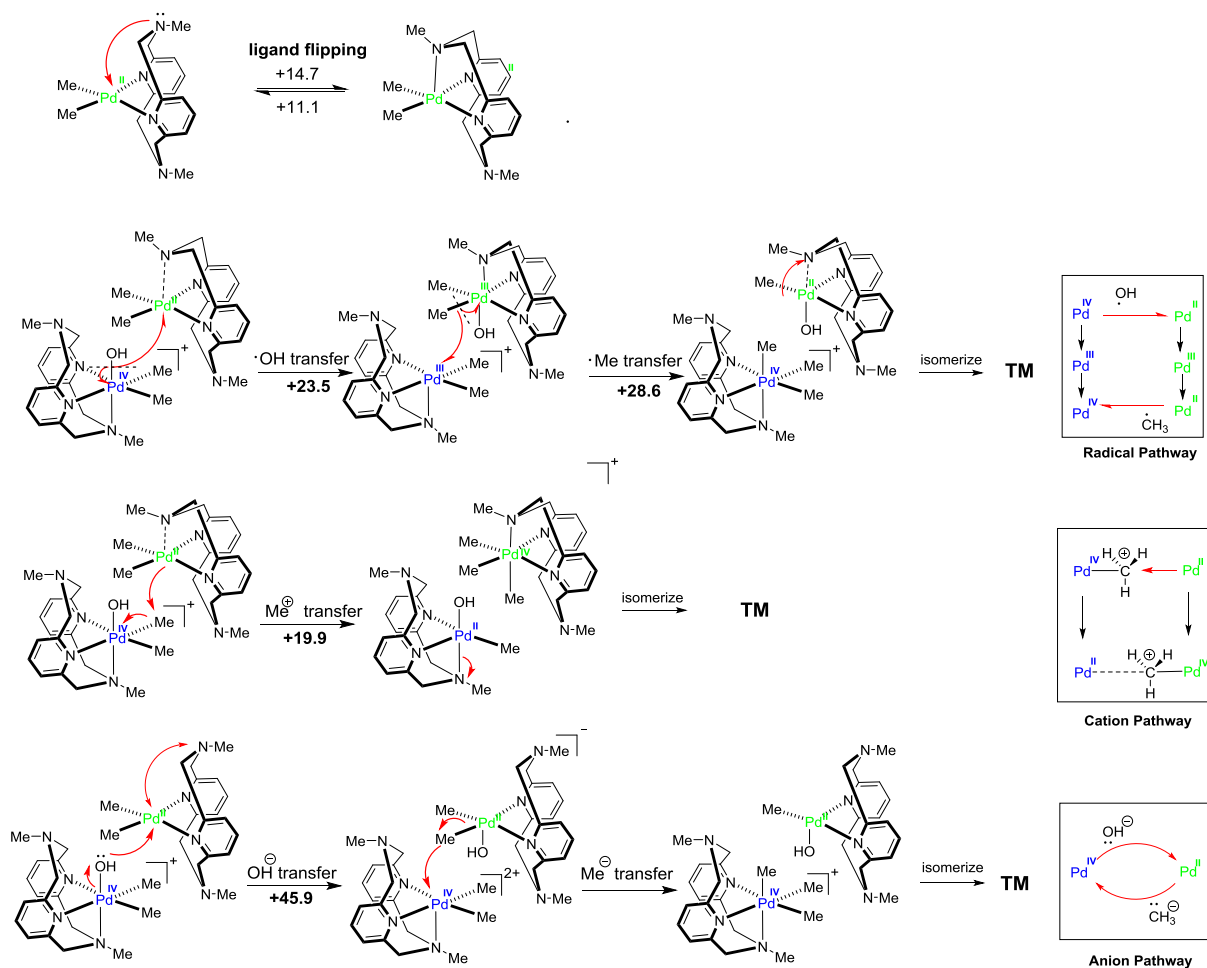


Table S2. The active energies of different functional and solvent corrections

All the calculations indicate the Me radical transfer is unfavorable.

Functional/sol-model	Reductive Elimination ΔG	Me ⁺ transfer ΔG	Me radical-transfer ΔG		
			Int- OH(T)	TS-OH(S)	TS-Me(T)
B3lyp/CPCM	23.3	30.4	37.3	40.2	57.8
B3lyp/SMD	23.3	33.0	40.6	44.1	61.3
B3lyp-D3/CPCM	24.5	17.5	20.2	22.6	43.2
B3lyp-D3/SMD	24.4	19.9	23.5	26.5	46.7
ω B97XD/CPCM	21.2	23.0	20.6	35.2	48.1
ω B97XD/SMD	21.1	25.6	24.1	39.3	51.8
M06L/CPCM	24.2	13.4	20.1	11.0	40.4
M06L/SMD	24.1	16.0	23.2	14.6	43.8

6-311++G**/Lanl2TZ basis set

Ligand flexibility of $(^{\text{Me}}\text{L})\text{Pd}^{\text{IV}}\text{Me}_2\text{X}$ complex

In Figure S6, the irreversible process is from $\kappa 2$ - to $\kappa 3$ - for $[(^{\text{Me}}\text{L})\text{Pd}^{\text{IV}}\text{Me}_2\text{X}]^+$, and the ligand can free flip between $\kappa 3$ - and $\kappa 4$ -. However, $[(^{\text{Me}}\text{L})\text{Pd}^{\text{IV}}\text{Me}_2]^ {2+}$ is highly stabilized by $\kappa 4$ - coordination, no ligand flipping could occur once $\kappa 4$ -complex formed.

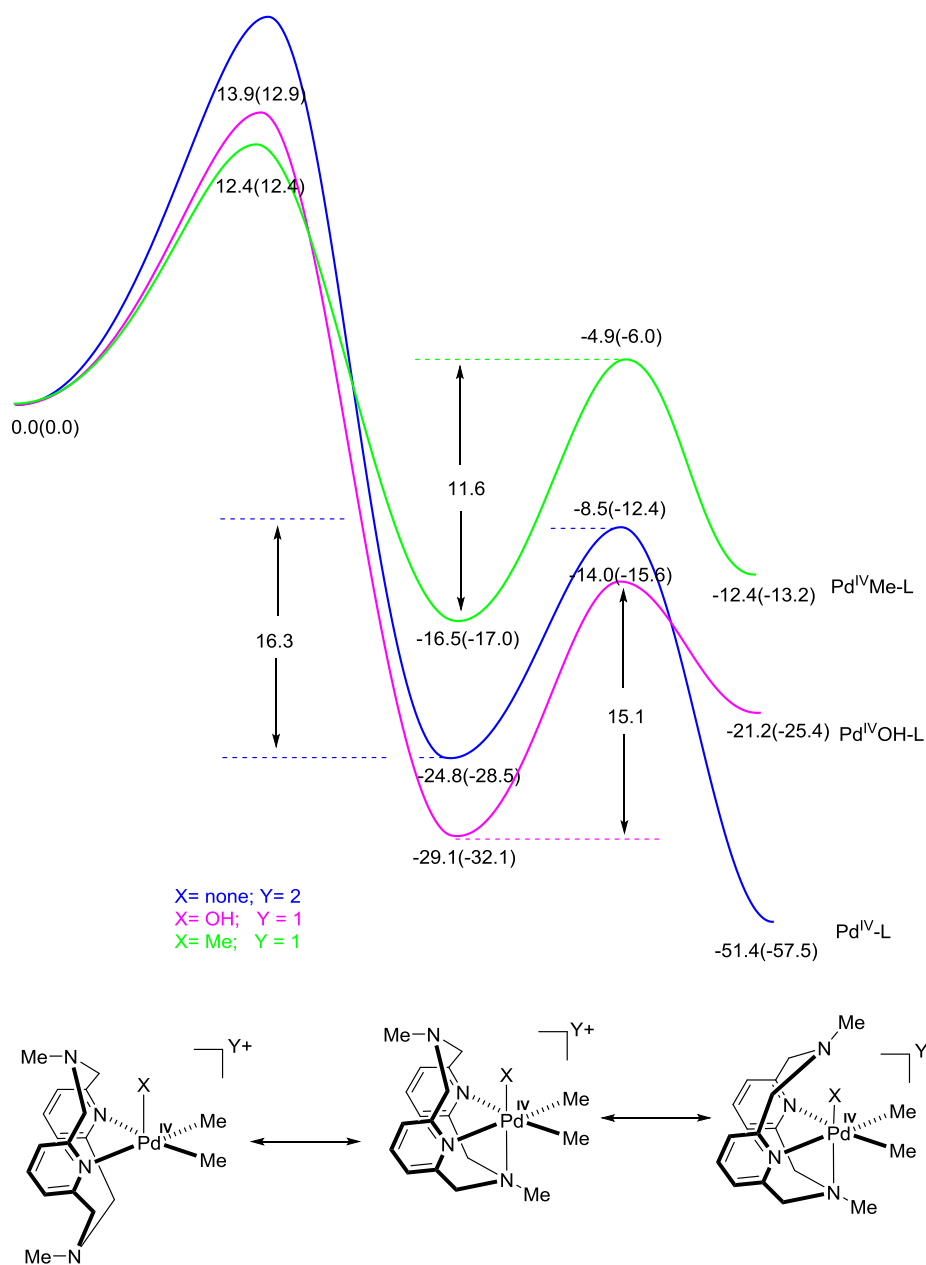


Figure S9. Energy profile of ligand flexibility of $(^{\text{Me}}\text{L})\text{Pd}^{\text{IV}}\text{Me}_2\text{X}$ complex at B3LYP/6-31G** level of theory.

Energy profiles of reductive elimination and ligand flexibility

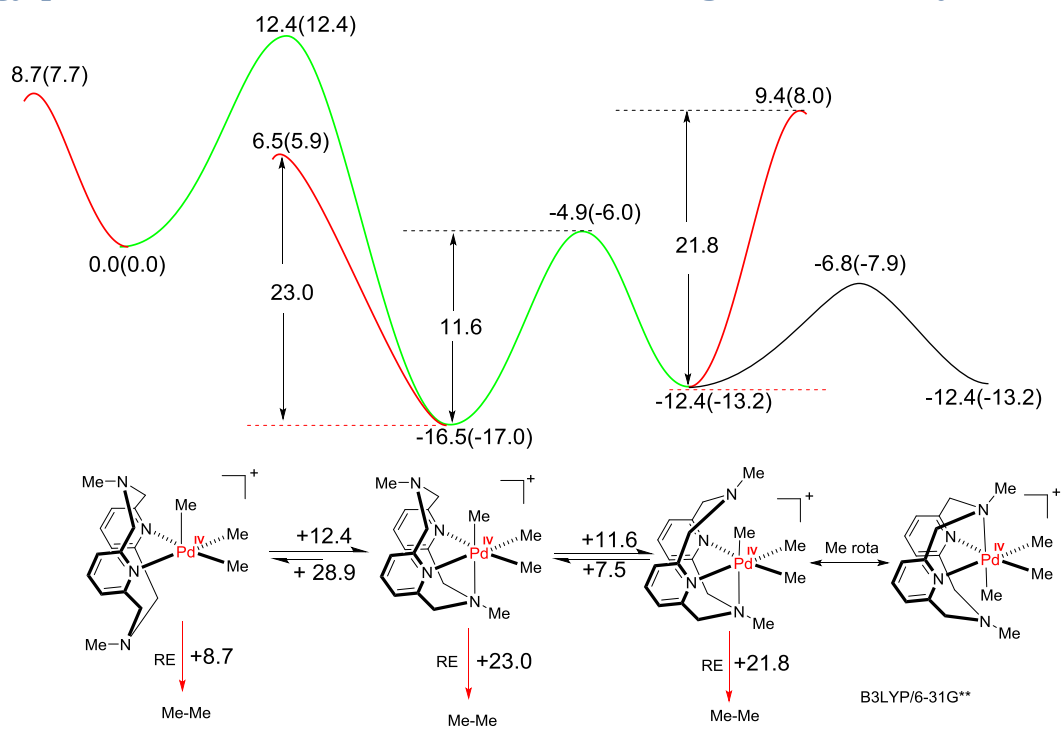


Figure S10. Energy profiles of reductive elimination and ligand flexibility at B3LYP/6-31G** level of theory

Table S3. Cartesian coordinates and imaginary frequency of the calculated structures

$\text{Me}_L(\text{N}_2, \text{TS}_{\text{N}_2\text{N}_3, \text{N}_3, \text{TS}_{\text{N}_3\text{N}_4, \text{N}_4})$				$\text{Me}_L_{\text{TS}_{\text{N}_2\text{N}_3}} \text{ frequency} = -147.43 \text{ cm}^{-1}$			
$\text{Me}_L_{\text{N}_2}$							
N	-0.0000285	-1.4346333	-1.0562310	N	-0.2129153	-1.7366314	-0.7349345
N	0.0000255	1.4346087	-1.0562250	N	0.2881117	0.9923386	-0.6198044
N	3.0384255	-0.0000313	-0.7237799	N	3.0460487	-0.3439144	-0.2665084
N	-3.0384315	0.0000147	-0.7237639	N	-2.9521713	-0.1677654	-0.9196834
C	-1.1581925	-1.7114423	-0.4404149	C	-1.3504853	-1.9066424	-0.0544314
C	-1.2002165	-2.3518103	0.8057761	C	-1.3612483	-2.1851953	1.3187676
H	-2.1523275	-2.5972893	1.2660841	H	-2.2991863	-2.3263294	1.8476606
C	-0.0000305	-2.6845043	1.4297861	C	-0.1391373	-2.2650404	1.9866736
H	-0.0000315	-3.1970343	2.3879631	H	-0.1073433	-2.4991214	3.0474616
C	1.2001515	-2.3517703	0.8058011	C	1.0396557	-2.0029434	1.2878176
H	2.1522625	-2.5971853	1.2661421	H	2.0057187	-1.9989984	1.7821616
C	1.1581335	-1.7114273	-0.4404049	C	0.9509897	-1.7126514	-0.0771614
C	2.4267555	-1.2585733	-1.1588480	C	2.1316607	-1.2831194	-0.9188654
H	3.1960385	-2.0357153	-1.0510320	H	2.7380477	-2.1692294	-1.1596814
H	2.1835255	-1.1651933	-2.2209120	H	1.7177287	-0.9084834	-1.8644575
C	2.4268095	1.2585487	-1.1588210	C	1.1716197	1.4752886	0.2532206
H	2.1836085	1.1652127	-2.2208960	C	0.8521537	2.5315237	1.1254286
H	3.1961165	2.0356577	-1.0509529	H	1.5904787	2.9035097	1.8304926
C	1.1581835	1.7114157	-0.4403979	C	-0.4158903	3.0907067	1.0616776
C	1.2001915	2.3517857	0.8057941	H	-0.6826773	3.9279287	1.7007876
H	2.1522995	2.5972037	1.2661411	C	-1.3503513	2.5455577	0.1804046
C	0.0000035	2.6845347	1.4297601	H	-2.3556743	2.9496567	0.1212526
H	-0.0000055	3.1970837	2.3879271	C	-0.9743653	1.4658486	-0.6241374
C	-1.2001775	2.3518327	0.8057471	C	-2.0010673	0.7772256	-1.5335304
H	-2.1522915	2.5973197	1.2660441	H	-2.6028093	1.5658786	-2.0089605
C	-1.1581445	1.7114357	-0.4404299	H	-1.4560923	0.2429136	-2.3135234
C	-2.4267685	1.2585597	-1.1588619	C	-2.5912293	-1.5906854	-0.8721024
H	-3.1960555	2.0357007	-1.0510579	H	-2.4030183	-1.9282884	-1.8965644
H	-2.1835465	1.1651557	-2.2209240	H	-3.4664443	-2.1287603	-0.4902474
C	-2.4268205	-1.2585653	-1.1588329	C	4.2416917	-0.1409634	-1.0733844
H	-2.1836305	-1.1652073	-2.2209060	C	-3.6803013	0.3236366	0.2340546
H	-3.1961275	-2.0356783	-1.0509750	H	-3.0795903	0.4523036	1.1511476
C	3.5817375	-0.0000513	0.6206061	H	-4.4985543	-0.3679014	0.4638096
H	2.8324155	-0.0000573	1.4308571	H	-4.1297583	1.2953216	-0.0041964
H	4.2150865	0.8851147	0.7546571	H	4.0580407	0.4110506	-2.0146705
H	4.2150785	-0.8852283	0.7546341	H	4.9975357	0.4069346	-0.5016484
C	-3.5816765	0.0000447	0.6206511	H	4.6736397	-1.1119054	-1.3382714
H	-2.8323165	-0.0000063	1.4308631	C	2.5873907	0.9001146	0.3780256
H	-4.2150755	-0.8850843	0.7547131	H	3.2606117	1.7047666	0.0533966
H	-4.2149535	0.8852597	0.7547201	H	2.7591857	0.8120636	1.4625256

$\text{Me}_L_{\text{N}_3}$				$\text{Me}_L_{\text{TS}_{\text{N}_3\text{N}_4}} \text{ frequency} = -129.34 \text{ cm}^{-1}$			
N	0.2048523	-1.4205522	-0.6651572	N	-0.2166220	-1.4434315	-0.2384002
N	2.7502293	-0.0000022	-0.8200902	N	2.9686790	-0.2012675	-0.7844062
N	-2.8096897	-0.0000012	-1.2729812	N	-2.5242211	-0.2725195	-1.0718782
C	-1.0832227	-1.6570062	-0.3855422	C	-1.1801921	-1.4371045	0.6776048
C	-1.4923337	-2.1749952	0.8528318	C	-0.9200761	-1.7359375	2.0219438
H	-2.5367166	-2.4082762	1.0346078	H	-1.7183351	-1.7253695	2.7592918
C	-0.5328567	-2.3800232	1.8405178	C	0.3935859	-2.0191355	2.3947648
H	-0.8156937	-2.7764722	2.8118628	H	0.6272260	-2.2673605	3.4265748
C	0.7935453	-2.0446652	1.5727738	C	1.4132690	-1.9268645	1.4445378
H	1.5608993	-2.1514742	2.3339098	H	2.4536670	-2.0740775	1.7178918
C	1.1219224	-1.5696182	0.2981438	C	1.0589780	-1.6046745	0.1314198
C	2.5627933	-1.2336762	-0.0602472	C	2.0433440	-1.3295095	-0.9841772
H	3.1731283	-1.2513682	0.8655968	H	2.6743339	-2.2161635	-1.1530682
H	2.9383403	-2.0506752	-0.6889102	H	1.4275570	-1.1896305	-1.8836622
C	-2.0819617	-1.2594362	-1.4697612	C	-2.5653501	-1.0152115	0.1832268
H	-1.5258177	-1.1853982	-2.4084142	H	-3.1590801	-1.9199425	0.0022138
H	-2.8409537	-2.0460002	-1.5793202	H	-3.0853551	-0.4772595	0.9997448
C	4.0301754	-0.0000032	-1.5160382	C	3.6769239	0.0690685	-2.0264352
H	4.9102724	-0.0000022	-0.8421412	H	4.1219980	-0.8596865	-2.4021562
H	4.0998914	0.8840558	-2.1570782	H	4.4958550	0.7743555	-1.8535622
C	-3.7791876	-0.0000012	-0.1943662	C	-3.7028811	-0.4726015	-1.8968232
H	-3.3532706	-0.0000012	0.8239168	H	-4.6303271	-0.0326435	-1.4765652

H	-4.4200896	0.8852908	-0.2849402	H	-3.8742360	-1.5424115	-2.0501202
N	0.2048523	1.4205498	-0.6651592	N	0.2149159	1.2463305	-0.5065062
C	-1.0832227	1.6570048	-0.3855442	C	-1.0355971	1.5406855	-0.1032812
C	-1.4923317	2.1749998	0.8528278	C	-1.3013390	2.1572195	1.1233788
H	-2.5367137	2.4082838	1.0346038	H	-2.3209351	2.4105175	1.3958378
C	-0.5328537	2.3800308	1.8405128	C	-0.2420540	2.4177395	1.9907008
H	-0.8156907	2.7764828	2.8118558	H	-0.4143731	2.8952535	2.9511978
C	0.7935463	2.0446698	1.5727698	C	1.0312240	2.0109025	1.6184418
H	1.5609014	2.1514808	2.3339038	H	1.8738929	2.1385915	2.2912478
C	1.1219233	1.5696188	0.2981408	C	1.2217010	1.4235655	0.3548458
C	2.5627943	1.2336738	-0.0602502	C	2.6481560	1.0089005	-0.0106882
H	3.1731294	1.2513678	0.8655948	H	3.1928019	0.9685645	0.9446678
H	2.9383424	2.0506708	-0.6889142	H	3.0850409	1.8575145	-0.5530932
C	-2.0819617	1.2594328	-1.4697622	C	-2.1931141	1.1606705	-1.0089002
H	-1.5258177	1.1853948	-2.4084152	H	-1.9534291	1.4736375	-2.0319082
H	-2.8409547	2.0459978	-1.5793212	H	-3.0744250	1.7507785	-0.6868762
H	4.0998903	-0.8840632	-2.1570762	H	3.0309250	0.4752895	-2.8270702
H	-4.4200896	-0.8852952	-0.2849402	H	-3.5421321	-0.0167825	-2.8799562

Me ₂ L-N ₄				Me ₂ L ^{II} Pd ^{II} Me ₂ (N ₂ ,TS-N ₂ N ₃ ,N ₃ ,TS-N ₃ N ₄ ,N ₄)			
N	0.3382476	-1.4199210	-0.0000000	Me ₂ L ^{II} Pd ^{II} Me ₂ -N ₂			
N	1.2195506	-0.0000000	2.3964740	Pd	-1.3047836	0.0336068	-1.5369219
N	1.2195506	-0.0000000	-2.3964740	N	-1.2523496	-0.0116522	0.7252811
C	-0.3297244	-1.5442110	-1.1513390	N	0.9192464	0.0202148	-1.1176619
C	-1.6746424	-1.9317030	-1.1989910	N	0.1351974	-2.9784102	0.1074701
H	-2.1832024	-2.0343220	-2.1530710	N	0.1482964	2.9709938	0.2264471
C	-2.3465654	-2.1587700	-0.0000000	C	-3.3384796	0.0457428	-1.7901409
H	-3.3887744	-2.4657930	-0.0000000	H	-3.6694526	1.0110348	-2.1905079
C	-1.6746424	-1.9317030	1.1989910	H	-3.8218856	-0.1148892	-0.8174139
H	-2.1832024	-2.0343220	2.1530710	H	-3.6649416	-0.7392752	-2.4801949
C	-0.3297244	-1.5442110	1.1513390	C	-1.2243446	0.0718858	-3.5844139
C	0.4420536	-1.2384430	2.4278810	H	-1.5865736	-0.8754232	-4.0003679
H	-0.2597484	-1.2703120	3.2861140	H	-0.1827216	0.2179218	-3.8996559
H	1.1585166	-2.0540380	2.5848450	H	-1.8348946	0.8812428	-3.9981499
C	0.4420536	-1.2384430	-2.4278810	C	-1.1698396	1.1427328	1.4202221
H	1.1585166	-2.0540380	-2.5848450	C	-1.0723846	1.1428108	2.8158671
H	-0.2597484	-1.2703120	-3.2861140	H	-1.0363896	2.0868898	3.3501141
C	2.2495856	-0.0000000	3.4257180	C	-1.0345326	-0.0687172	3.5001661
H	1.8534176	-0.0000000	4.4612750	H	-0.9706866	-0.0909292	4.5844021
H	2.8840196	0.8841630	3.3107510	C	-1.0784396	-1.2511452	2.7671801
C	2.2495856	-0.0000000	-3.4257180	H	-1.0471216	-2.2163652	3.2625251
H	1.8534176	-0.0000000	-4.4612750	C	-1.1756026	-1.1937282	1.3726421
H	2.8840196	-0.8841620	-3.3107510	C	-1.1687786	-2.4685642	0.5344201
N	0.3382456	1.4199200	-0.0000000	H	-1.6451696	-3.2632832	1.1247211
C	-0.3297244	1.5442090	-1.1513390	H	-1.7744436	-2.2918902	-0.3597509
C	-1.6746424	1.9317030	-1.1989920	C	0.7615454	-2.4406252	-1.1011989
H	-2.1832024	2.0343240	-2.1530710	H	-0.0237506	-2.2684712	-1.8435379
C	-2.3465664	2.1587720	-0.0000000	H	1.4364724	-3.2181482	-1.4844719
H	-3.3887744	2.4657960	-0.0000000	C	1.5664654	-1.1529612	-0.9529579
C	-1.6746424	1.9317030	1.1989920	C	2.9273774	-1.1905732	-0.6307249
H	-2.1832024	2.0343240	2.1530710	H	3.4281714	-2.1484702	-0.5325479
C	-0.3297244	1.5442090	1.1513390	C	3.6224084	0.0020888	-0.4518989
C	0.4420526	1.2384420	2.4278810	H	4.6820784	-0.0046242	-0.2127469
H	-0.2597504	1.2703110	3.2861130	C	2.9319964	1.2034268	-0.5840139
H	1.1585146	2.0540370	2.5848450	H	3.4363914	2.1548558	-0.4484899
C	0.4420526	1.2384420	-2.4278810	C	1.5708704	1.1835428	-0.9071419
H	1.1585146	2.0540370	-2.5848450	C	0.7703284	2.4787938	-1.0037499
H	-0.2597504	1.2703110	-3.2861130	H	1.4471334	3.2683858	-1.3579649
H	2.8840196	-0.8841620	3.3107510	H	-0.0171836	2.3379418	-1.7504579
H	2.8840196	0.8841630	-3.3107510	C	-1.1574536	2.4507928	0.6348671
				H	-1.7658056	2.3145088	-0.2644269
				H	-1.6284726	3.2230948	1.2582951
				C	1.0405214	-3.3699982	1.1690901
				H	1.5005854	-2.5350392	1.7263421
				H	1.8526624	-3.9752782	0.7489791
				H	0.5032854	-3.9949192	1.8924761
				C	1.0568704	3.3158838	1.3013941
				H	1.5137924	2.4573228	1.8243061

	H	0.5235194	3.9140218	2.0498591
	H	1.8712664	3.9336418	0.9044421
Me₂LPd^{II}Me₂_TS_N₂N₃ frequency=-250.34 cm⁻¹				
Pd	1.0986793	-1.4129167	0.0150036	
N	-0.0427707	0.0234723	1.3615886	
N	2.5352713	1.4601383	-0.0213594	
C	2.0453033	-2.5986987	-1.3592724	
H	3.1250483	-2.6379557	-1.1797974	
H	1.8669703	-2.1912297	-2.3631264	
H	1.6544603	-3.6218367	-1.3217914	
C	-1.3374827	-0.2164387	1.6554826	
C	-2.1473607	0.7721003	2.2304576	
H	-3.1695127	0.5353553	2.5067486	
C	-1.6302317	2.0470593	2.4307836	
H	-2.2431627	2.8325693	2.8634576	
C	-0.3092357	2.2980903	2.0664796	
H	0.1308023	3.2805933	2.2009916	
C	0.4683163	1.2594303	1.5461526	
C	1.9519553	1.4666773	1.3162496	
H	2.2168803	2.4099583	1.8265036	
H	2.4325303	0.6606383	1.8916566	
C	-1.9077637	-1.5801527	1.2792406	
H	-1.0761427	-2.2878687	1.2084296	
H	-2.5856497	-1.9128327	2.0758936	
C	3.9433693	1.1083053	-0.0170674	
H	4.4413973	1.5490213	0.8543306	
H	4.4389123	1.5184143	-0.9045784	
N	-0.0470947	-0.0086277	-1.3613054	
C	-1.3430647	-0.2539457	-1.6447954	
C	-2.1535247	0.7216353	-2.2405774	
H	-3.1770457	0.4799313	-2.5073814	
C	-1.6349977	1.9904453	-2.4741804	
H	-2.2483357	2.7660143	-2.9238774	
C	-0.3121547	2.2481783	-2.1214514	
H	0.1291303	3.2261873	-2.2821374	
C	0.4654093	1.2212983	-1.5782674	
C	1.9501953	1.4298703	-1.3578884	
H	2.2174473	2.3571903	-1.8954194	
H	2.4264773	0.6055313	-1.9104134	
C	-1.9127307	-1.6083157	-1.2353314	
H	-1.0809417	-2.3144677	-1.1520934	
H	-2.5938057	-1.9584917	-2.0217004	
H	4.1115703	0.0181053	0.0014916	
C	2.0511673	-2.5677387	1.4121486	
H	3.1234343	-2.3386917	1.4235366	
H	1.6340453	-2.3443027	2.4028826	
H	1.9318903	-3.6373827	1.2115806	
N	-2.6658797	-1.6407537	0.0239306	
C	-3.9246707	-0.9201257	0.0181786	
H	-4.5066357	-1.2171617	-0.8621874	
H	-4.5031377	-1.1968297	0.9074286	
H	-3.8373287	0.1805543	0.0053706	
Me₂LPd^{II}Me₂_TS_N₃N₄ frequency=-256.65 cm⁻¹				
Pd	1.0809305	-1.1246592	-0.0587341	
N	-0.1636045	0.2421968	1.3614029	
N	2.1682365	1.4365118	0.0217299	
N	-1.9029755	-2.1030312	-0.0403251	
C	1.9899665	-2.2701602	-1.4917901	
H	3.0811465	-2.1956862	-1.4140131	
H	1.6825505	-1.9015712	-2.4799621	
H	1.7125755	-3.3265442	-1.4090301	
C	-1.4486215	-0.1252242	1.5538319	
C	-2.4048515	0.7734618	2.0381509	
H	-3.4254005	0.4378158	2.1897679	
C	-2.0315215	2.0853358	2.3145289	
H	-2.7544345	2.7997868	2.6974789	
C	-0.7182125	2.4691968	2.0623449	
H	-0.3925705	3.4911938	2.2291919	
C	0.1880215	1.5262568	1.5672489	
C	1.6231565	1.9399608	1.2749609	
Me₂LPd^{II}Me₂_N₄				
Pd	-1.6142468	0.0013883	0.0000001	
N	0.3492492	-0.0003097	1.3661771	
N	-0.4566248	-2.4984967	-0.0000159	
N	-0.4523128	2.4992563	0.0000161	
C	-3.1360488	0.0027223	-1.3719219	
H	-2.6874468	0.0013093	-2.3754499	
H	-3.7700318	0.8913763	-1.2729169	
H	-3.7728988	-0.8837307	-1.2717129	
C	1.0136542	1.1587453	1.5507331	
C	2.3241292	1.1927333	2.0372771	
H	2.8180712	2.1485073	2.1820421	
C	2.9824192	-0.0026017	2.3086441	
H	4.0006092	-0.0034887	2.6867051	
C	2.3220532	-1.1967887	2.0372681	
H	2.8143322	-2.1534217	2.1820271	
C	1.0116382	-1.1605207	1.5507251	
C	0.2934252	-2.4681187	1.2474001	

H	1.6885455	3.0425028	1.3575429	H	1.0319302	-3.2902417	1.3242281
H	2.2526215	1.5304168	2.0744959	H	-0.4381268	-2.6315627	2.0483771
C	-1.8234155	-1.5729772	1.3136739	C	0.2977132	2.4675933	1.2474131
H	-1.0600905	-2.1588342	1.8483609	H	-0.4335288	2.6323223	2.0484101
H	-2.7791425	-1.7459072	1.8427429	H	1.0376522	3.2884283	1.3242121
C	3.6257595	1.4323618	0.0134069	C	-1.4865328	-3.5296177	-0.0000259
H	4.0704065	2.4455668	0.0257139	H	-1.0810078	-4.5593657	0.0000121
H	3.9811855	0.9099208	-0.8787741	H	-2.1211398	-3.4065237	-0.8814709
C	-1.7733425	-3.5472682	-0.0778171	C	-1.4805148	3.5320763	0.0000271
H	-2.1586295	-3.9364432	-1.0256411	H	-1.0732948	4.5611553	-0.0000119
H	-0.7288605	-3.8809582	0.0364109	H	-2.1153268	3.4100243	0.8814701
N	-0.2038535	0.3222798	-1.3388421	N	0.3492492	-0.0002947	-1.3661769
C	-1.5004245	-0.0137472	-1.5075911	C	1.0136422	1.1587693	-1.5507289
C	-2.4564555	0.9279978	-1.9035291	C	2.3241162	1.1927723	-2.0372729
H	-3.4875975	0.6183768	-2.0377421	H	2.8180482	2.1485523	-2.1820339
C	-2.0700655	2.2476328	-2.1171261	C	2.9824192	-0.0025547	-2.3086449
H	-2.7932735	2.9941938	-2.4322121	H	4.0006092	-0.0034287	-2.6867049
C	-0.7422465	2.5955438	-1.8899861	C	2.3220652	-1.1967497	-2.0372729
H	-0.4042425	3.6201438	-2.0089521	H	2.8143552	-2.1533757	-2.1820359
C	0.1628805	1.6113598	-1.4814331	C	1.0116502	-1.1604967	-1.5507289
C	1.6124115	1.9831808	-1.2093551	C	0.2934482	-2.4681047	-1.2474179
H	1.7031245	3.0856668	-1.2647421	H	1.0319642	-3.2902197	-1.3242399
H	2.2171325	1.5776358	-2.0296891	H	-0.4380888	-2.6315527	-2.0484069
C	-1.8983785	-1.4686942	-1.3518661	C	0.2976902	2.4676073	-1.2473949
H	-1.1887995	-2.0240192	-1.9821951	H	-0.4335658	2.6323333	-2.0483799
H	-2.8903225	-1.5724472	-1.8292391	H	1.0376192	3.2884513	-1.3242009
H	3.9914445	0.8840808	0.8857079	H	-2.1211998	-3.4064767	0.8813691
H	-2.3725325	-4.0076582	0.7194419	H	-2.1153878	3.4099773	-0.8813669
C	2.0486495	-2.3504842	1.2651899	C	-3.1360488	0.0027893	1.3719221
H	3.1287595	-2.1618462	1.2348279	H	-2.6874458	0.0025053	2.3754501
H	1.6831565	-2.1305442	2.2776629	H	-3.7707088	0.8908773	1.2722231
H	1.8812025	-3.4118712	1.0547719	H	-3.7722238	-0.8842317	1.2724061
[^{Me} LPd ^{III} Me ₂] ⁺ (N ₂ ,TS_N ₂ N ₃ ,N ₃ ,TS_N ₃ N ₄ ,N ₄)				[^{Me} LPd ^{III} Me ₂] ⁺ _TS_N ₂ N ₃ frequency=-343.63 cm ⁻¹			
[^{Me} LPd ^{III} Me ₂] ⁺ _N ₂							
Pd	-0.0007637	1.9842688	-0.0000712	Pd	-0.5713765	1.7041875	0.0170153
N	0.0020613	0.2560508	-1.4320192	N	0.0642285	0.0238025	1.3793243
N	-0.0022397	0.2561528	1.4320008	N	-2.8614385	-0.6923515	-0.0109597
N	2.9726583	-0.1792242	0.0044518	N	3.0587315	0.7497065	0.0117753
N	-2.9725007	-0.1815122	-0.0044382	C	-1.1305725	3.0788195	-1.3986217
C	0.0008323	3.4406938	-1.4507032	H	-2.2105655	3.2207785	-1.2988987
H	-0.9010747	4.0410938	-1.3072732	H	-0.8778995	2.6725215	-2.3799327
H	0.0030923	2.9587098	-2.4293862	H	-0.6006305	4.0159925	-1.2149377
H	0.9011583	4.0426278	-1.3038442	C	1.3681155	-0.1712905	1.6578113
C	-0.0035337	3.4407958	1.4504558	C	1.8099085	-1.3702885	2.2288693
H	0.8978793	4.0419238	1.3069698	H	2.8548615	-1.4883635	2.4943793
H	-0.0053867	2.9588808	2.4291728	C	0.8969955	-2.3968095	2.4499183
H	-0.9043537	4.0419838	1.3035658	H	1.2186275	-3.3365345	2.8879673
C	-1.1687007	-0.3102202	-1.7908212	C	-0.4405535	-2.1970065	2.1089683
C	-1.1957417	-1.4577932	-2.5874102	H	-1.1790945	-2.9751535	2.2680203
H	-2.1474717	-1.8812272	-2.8902912	C	-0.8322515	-0.9653265	1.5836443
C	0.0052803	-2.0331252	-2.9959452	C	-2.2915145	-0.6458665	1.3472463
H	0.0065653	-2.9154862	-3.6284102	H	-2.8746325	-1.3625475	1.9404763
C	1.2046313	-1.4568632	-2.5838302	H	-2.4748795	0.3380655	1.8061013
H	2.1575883	-1.8795622	-2.8838652	C	2.3472815	0.9330015	1.2693003
C	1.1743243	-0.3093072	-1.7873342	H	1.7930915	1.8815335	1.2154843
C	2.4612603	0.3213188	-1.2615972	H	3.1005405	1.0336385	2.0588283
H	3.2463403	0.1714628	-2.0124272	C	-4.2797845	-0.3633765	-0.0093187
H	2.3022483	1.4047858	-1.1620692	H	-4.7641285	-0.7989875	0.8700053
C	2.4574663	0.3214018	1.2689278	H	-4.7618335	-0.7802455	-0.8989267
H	2.2987553	1.4048618	1.1688458	C	4.1474575	-0.2126745	0.0031913
H	3.2402913	0.1715998	2.0221198	H	3.8221515	-1.2662615	-0.0082067
C	1.1689583	-0.3091882	1.7908448	H	4.7735855	-0.0442635	-0.8788197
C	1.1968833	-1.4566822	2.5875188	N	0.0678535	0.0526165	-1.3784237
H	2.1489383	-1.8793592	2.8904338	C	1.3724545	-0.1367375	-1.6575117
C	-0.0036947	-2.0329132	2.9960918	C	1.8156975	-1.3236255	-2.2522507
H	-0.0042997	-2.9152292	3.6286198	H	2.8613385	-1.4362465	-2.5174257
C	-1.2034907	-1.4576082	2.5839308	C	0.9033245	-2.3452345	-2.4970187
H	-2.1561217	-1.8810222	2.8839928	H	1.2260665	-3.2756625	-2.9537027
C	-1.1740667	-0.3100862	1.7873538	C	-0.4351095	-2.1524565	-2.1554877
C	-2.4614887	0.3195128	1.2615748	H	-1.1732615	-2.9270525	-2.3326487

H	-3.2464517	0.1691058	2.0124148	C	-0.8281275	-0.9319535	-1.6056407
H	-2.3033067	1.4030938	1.1619678	C	-2.2879755	-0.6173145	-1.3664007
C	-2.4576937	0.3194158	-1.2689512	H	-2.8696075	-1.3212535	-1.9761147
H	-2.2998137	1.4030048	-1.1689472	H	-2.4700345	0.3760955	-1.8048957
H	-3.2404027	0.1689568	-2.0221322	C	2.3506005	0.9591675	-1.2435347
C	3.5563263	-1.5086762	0.0053708	H	1.7962605	1.9063955	-1.1714467
H	2.8167153	-2.3261142	0.0042828	H	3.1059365	1.0761775	-2.0288097
H	4.1891413	-1.6285812	0.8908358	H	-4.4723585	0.7222105	0.0019333
H	4.1918013	-1.6286342	-0.8781792	H	4.7712545	-0.0626815	0.8901643
C	-3.5551777	-1.5113982	-0.0052622	C	-1.1347695	3.0487435	1.4596163
H	-2.8149567	-2.3282832	-0.0041142	H	-2.2147215	3.1915195	1.3605463
H	-4.1879017	-1.6318402	-0.8907192	H	-0.8837075	2.6224855	2.4328403
H	-4.1905637	-1.6317662	0.8782968	H	-0.6055365	3.9901075	1.2965083
[^{Me} LPd ^{III} Me ₂] ⁺ _N ₃				[^{Me} LPd ^{III} Me ₂] ⁺ _TS_N ₃ N ₄ frequency=-338.14 cm ⁻¹			
Pd	1.3788301	-0.5532976	-0.8231488	Pd	-0.9498735	-1.1344681	-0.0151684
N	-0.0118289	-1.1068866	0.8610942	N	0.1846185	0.2903199	-1.3588074
N	2.1043401	0.8388814	0.8903202	N	-2.2951545	0.7836589	-0.0007114
N	-2.3104439	-1.3733316	-1.5543228	N	2.3853235	-1.7047931	-0.0095844
C	2.5433721	0.0799874	-2.3930608	C	-1.8856005	-2.3228291	1.3735886
H	3.6076941	0.0477724	-2.1569088	H	-1.6554275	-1.9099991	2.3595086
H	2.2348841	1.0990664	-2.6419668	H	-1.4707525	-3.3308111	1.2826206
H	2.3382601	-0.5873796	-3.2358808	H	-2.9646245	-2.3578771	1.2150606
C	-1.1857499	-1.7482766	0.6932562	C	1.5125475	0.1780139	-1.5547924
C	-2.0843509	-1.8760906	1.7582942	C	2.2592635	1.2619089	-2.0263374
H	-3.0067089	-2.4297926	1.6201222	H	3.3253435	1.1487859	-2.1899684
C	-1.7848099	-1.2843616	2.9825612	C	1.6193215	2.4723099	-2.2851324
H	-2.4716949	-1.3696516	3.8187602	H	2.1800645	3.3215129	-2.6628044
C	-0.5972599	-0.5656266	3.1169032	C	0.2525985	2.5846509	-2.0345684
H	-0.3454179	-0.0714616	4.0495032	H	-0.2717525	3.5198559	-2.2008474
C	0.2721891	-0.5012216	2.0288232	C	-0.4320375	1.4699839	-1.5507984
C	1.6152511	0.1939654	2.1396842	C	-1.9151645	1.5123979	-1.2412404
H	1.5912531	0.9261314	2.9589152	H	-2.2618605	2.5541939	-1.1920094
H	2.3608281	-0.5607716	2.4115132	H	-2.4547035	1.0315589	-2.0637934
C	-1.5225179	-2.2617276	-0.7045238	C	2.1403795	-1.1835831	-1.3540954
H	-0.5886679	-2.5014526	-1.2259018	H	1.4886595	-1.8874751	-1.8995114
H	-2.0873859	-3.1960066	-0.6014278	H	3.0948845	-1.1760791	-1.9030784
C	3.5793231	0.9788544	0.9430402	C	-3.7459275	0.4884889	-0.0077254
H	3.8838591	1.6427024	1.7638072	H	-4.3383785	1.4137649	-0.0005884
H	3.9391681	1.3911294	0.0000052	H	-3.9991475	-0.1034401	0.8723786
C	-3.6860909	-1.1446496	-1.1454358	C	2.8048115	-3.0965531	-0.0254234
H	-3.8074029	-0.4731336	-0.2787778	H	3.4282315	-3.2945191	-0.9038464
H	-4.2454709	-0.7156556	-1.9834978	H	1.9607265	-3.8077371	-0.0424594
N	-0.1589289	1.0931254	-0.8640448	N	0.1736975	0.2615909	1.3638836
C	-1.3684479	0.9843784	-1.4496188	C	1.4990535	0.1403579	1.5711926
C	-2.3416119	1.9716734	-1.2590508	C	2.2440945	1.2107219	2.0749076
H	-3.2956339	1.8918344	-1.7688438	H	3.3080035	1.0904779	2.2473826
C	-2.0741729	3.0430064	-0.4108598	C	1.6048095	2.4170689	2.3538776
H	-2.8184639	3.8161684	-0.2478658	H	2.1639375	3.2557989	2.7565256
C	-0.8425539	3.1022554	0.2406802	C	0.2411285	2.5395569	2.0915276
H	-0.6117129	3.9101114	0.9273002	H	-0.2819745	3.4725379	2.2735106
C	0.0978801	2.1051354	-0.0149518	C	-0.4419135	1.4382589	1.5758206
C	1.4837411	2.1600374	0.5980502	C	-1.9222115	1.4917039	1.2538636
H	1.4672311	2.7793034	1.5058042	H	-2.2641265	2.5356339	1.2179546
H	2.1452661	2.6623464	-0.1157248	H	-2.4705375	1.0008369	2.0645746
C	-1.6552189	-0.2764796	-2.2613058	C	2.1229015	-1.2189411	1.3448696
H	-0.7125429	-0.6479766	-2.6793178	H	1.4594305	-1.9333931	1.8617966
H	-2.3007529	-0.0037076	-3.1047888	H	3.0694145	-1.2308801	1.9073876
H	4.0323061	-0.0016596	1.0919382	H	-3.9947775	-0.0871841	-0.8999484
H	-4.1527049	-2.1032956	-0.8953228	H	3.4131905	-3.3190181	0.8576056
C	2.6908561	-2.1264306	-0.6629358	C	-1.8773225	-2.2926271	-1.4335844
H	3.7313601	-1.8023016	-0.7062768	H	-1.8399705	-1.7451091	-2.3793394
H	2.4843561	-2.6324926	0.2841132	H	-1.2956165	-3.2162751	-1.5153574
H	2.4862961	-2.8027456	-1.4987288	H	-2.9075795	-2.5323601	-1.1683154
[^{Me} LPd ^{III} Me ₂] ⁺ _N ₄				[^{Me} LPd ^{IV} Me ₃] ⁺ (N ₂ _TS_N ₂ N ₃ ,N ₃ _TS_N ₃ N ₄ ,N ₄)			
Pd	-0.7891711	-0.0000015	-1.1208082	Pd	1.8734401	-0.4382271	0.0305879
N	0.2244709	1.3788845	0.3188198	N	0.0521931	0.0163069	-1.4343021
N	1.5974859	0.0000015	-1.7959592	N	0.0213511	-0.0574581	1.4250799
C	-1.6634041	-1.3937665	-2.3623372	N	-1.3290719	-2.7266311	-0.0439481
H	-1.3977531	-2.3844195	-1.9809822	N	0.3852391	2.9932159	0.0492639

H	-1.2920191	-1.2760885	-3.3830962	C	3.4202381	0.1196399	-1.2104841
H	-2.7493031	-1.2733495	-2.3607082	H	3.6666031	1.1222639	-0.8519331
C	1.5378139	1.6080095	0.1557518	H	3.0033791	0.1380309	-2.2185261
C	2.2994159	2.1839455	1.1740508	H	4.3024971	-0.5136771	-1.1647591
H	3.3573459	2.3741395	1.0258198	C	3.1828371	-0.5678541	1.6006839
C	1.6782209	2.4930855	2.3838338	H	4.2219091	-0.5984261	1.2759979
H	2.2468569	2.9430385	3.1915638	H	2.9289331	-1.4609211	2.1744329
C	0.3298109	2.1839625	2.5606328	H	2.9909611	0.3287119	2.1948399
H	-0.1665351	2.3741665	3.5065848	C	-0.1855569	1.3074699	-1.7723571
C	-0.3719731	1.6080295	1.5002228	C	-1.2851599	1.6688019	-2.5560651
C	-1.8428291	1.2447615	1.6054738	H	-1.4234249	2.7086909	-2.8321701
H	-2.1380291	1.2055815	2.6651138	C	-2.1791969	0.6922019	-2.9804821
H	-2.4180111	2.0563275	1.1462938	H	-3.0291399	0.9488099	-3.6052531
C	2.1329689	1.2447505	-1.1934272	C	-1.9590379	-0.6208251	-2.5807641
H	1.8946979	2.0563305	-1.8897612	H	-2.6364809	-1.4133551	-2.8800651
C	3.2300849	1.2055765	-1.1139292	C	-0.8457969	-0.9332401	-1.7937781
C	-3.6810581	-0.0000055	0.6262318	C	-0.6742949	-2.3671201	-1.2979881
H	-4.2750851	-0.0000085	1.5522008	H	-1.0801249	-3.0323281	-2.0697791
H	-3.9392161	-0.8849395	0.0421098	H	0.3853681	-2.5971171	-1.2096991
C	1.8313149	0.0000015	-3.2542142	C	-0.6882709	-2.4214701	1.2297359
H	2.9034179	0.0000045	-3.5009712	H	0.3800571	-2.6297511	1.1411439
H	1.3685829	0.8849415	-3.6943432	H	-1.0901499	-3.1234611	1.9704799
N	0.2244759	-1.3788835	0.3188208	C	-0.8724409	-1.0097251	1.7738159
C	1.5378199	-1.6080035	0.1557538	C	-1.9739559	-0.7071431	2.5797819
C	2.2994229	-2.1839355	1.1740548	H	-2.6567269	-1.4986881	2.8695939
H	3.3573529	-2.3741255	1.0258248	C	-2.1719449	0.6000709	3.0123189
C	1.6782279	-2.4930775	2.3838368	H	-3.0116099	0.8509439	3.6530999
H	2.2468659	-2.9430285	3.1915668	C	-1.2712179	1.5797799	2.6058219
C	0.3298169	-2.1839595	2.5606348	H	-1.3937329	2.6119789	2.9159189
H	-0.1665291	-2.3741655	3.5065868	C	-0.1871479	1.2265569	1.7978479
C	-0.3719681	-1.6080305	1.5002238	C	0.7581881	2.3094119	1.2801969
C	-1.8428261	-1.2447675	1.6054728	H	0.8546831	3.0721759	2.0633679
H	-2.1380281	-1.2055905	2.6651118	H	1.7588501	1.8829709	1.1363059
H	-2.4180041	-2.0563345	1.1462908	C	0.7336441	2.4016159	-1.2372131
C	2.1329749	-1.2447425	-1.1934242	H	1.7546591	2.0226109	-1.1684911
H	1.8947099	-2.0563255	-1.8897582	H	0.7488341	3.2153999	-1.9718851
C	3.2300909	-1.2055625	-1.1139242	C	-2.7821889	-2.7223541	-0.0475721
H	-3.9392191	0.8849305	0.0421138	H	-3.2451429	-1.7218681	-0.0245051
H	1.3685899	-0.8849435	-3.6943412	H	-3.1470629	-3.2807921	0.8211659
C	-1.6634001	1.3937585	-2.3623452	H	-3.1426269	-3.2382951	-0.9438151
H	-1.3976561	2.3844135	-1.9810582	C	-0.8258619	3.7951679	0.0920749
H	-1.2920991	1.2760075	-3.3831262	H	-1.7649429	3.2178909	0.0828199
H	-2.7493061	1.2734115	-2.3606282	H	-0.8391229	4.4734109	-0.7674241
				H	-0.8188729	4.4119549	0.9971409
				C	2.6941251	-2.2835271	-0.4721011
				H	2.5481231	-2.4072871	-1.5443411
				H	3.7441431	-2.3583581	-0.2052391
				H	2.1000491	-2.9861831	0.1114249
[^{Me} LPd ^{IV} Me ₃] ⁺ TS_N ₂ N ₃ frequency=311.18 cm ⁻¹				[^{Me} LPd ^{IV} Me ₃] ⁺ N ₃			
Pd	-1.2403196	-1.2325517	-0.0411721	Pd	-1.4477325	-0.9048513	-0.0000146
N	0.1710684	0.0742743	1.3732139	N	0.2138065	0.1142887	-1.3977436
N	0.2104814	0.1024943	-1.3799581	N	-2.0242735	1.3488997	0.0000324
N	2.7572094	-1.6696557	-0.0123971	N	2.5953825	-1.8016023	-0.0000406
N	-2.2356866	1.8858473	-0.0022701	C	-2.7866075	-1.3807183	1.4771244
C	-2.8162626	-1.6034767	1.2173439	H	-3.6823965	-1.8576923	1.0822584
H	-3.4944846	-0.7822337	0.9715249	H	-3.0366765	-0.4323453	1.9558214
H	-2.4290816	-1.5201927	2.2337809	H	-2.2856865	-2.0368433	2.1889794
H	-3.3087966	-2.5605267	1.0622329	C	-1.2132495	-2.9763573	-0.0000536
C	-2.3658476	-1.9621897	-1.5813471	H	-2.1889925	-3.4598233	-0.0000456
H	-3.0464946	-2.7588957	-1.2876651	H	-0.6699425	-3.2694723	-0.8981186
H	-1.6643806	-2.3065147	-2.3437241	C	1.4422355	-0.3458223	-1.7253686
H	-2.9302576	-1.0965867	-1.9379021	C	2.3591995	0.4599357	-2.4121766
C	-0.2654306	1.3401493	1.5813139	H	3.3178505	0.0442627	-2.7027776
C	0.5719964	2.3322463	2.0942709	C	2.0376325	1.7798337	-2.7050036
H	0.1828984	3.3327993	2.2471029	H	2.7373805	2.4190297	-3.2342426
C	1.8852794	2.0146543	2.4302919	C	0.8054215	2.2715867	-2.2830946
H	2.5434904	2.7613833	2.8634069	H	0.5266555	3.3054687	-2.4580316
C	2.3303964	0.7193333	2.2013389	C	-0.0813235	1.4095777	-1.6374496
H	3.3437344	0.4273623	2.4538789	C	-1.4504395	1.9217577	-1.2452096

C	1.4647234	-0.2249227	1.6344599	H	-1.4273755	3.0191177	-1.1836366
C	2.0073954	-1.5946627	1.2427459	H	-2.1469135	1.6728117	-2.0533786
C	2.6833354	-1.9365927	2.0346849	C	1.8631745	-1.7361063	-1.2628046
H	1.1850174	-2.3053577	1.1972389	H	0.9832415	-2.3709743	-1.1853366
C	2.0252794	-1.5706327	-1.2747381	H	2.5128915	-2.1689813	-2.0327166
H	1.1845764	-2.2673427	-1.2511721	C	-3.4836495	1.6304927	0.0000174
H	2.7035234	-1.9120137	-2.0650581	H	-3.6753385	2.7119827	0.0000394
C	1.5020444	-0.1892447	-1.6446491	H	-3.9474665	1.1937517	0.8845664
C	2.3666974	0.7698373	-2.1871501	C	3.9351945	-1.2398973	-0.0000236
H	3.3824494	0.4894873	-2.4432701	H	3.9815815	-0.1377163	0.0000004
C	1.9133454	2.0676093	-2.3887551	H	4.4758295	-1.5975953	0.8827944
H	2.5694284	2.8270383	-2.8026041	N	0.2138125	0.1142317	1.3977454
C	0.5954284	2.3727703	-2.0559131	C	1.4422415	-0.3458953	1.7253464
H	0.2015274	3.3735463	-2.1947831	C	2.3592115	0.4598317	2.4121804
C	-0.2384356	1.3661383	-1.5669821	H	3.3178635	0.0441447	2.7027574
C	-1.7089496	1.6504303	-1.3498791	C	2.0376485	1.7797177	2.7050674
H	-1.9437216	2.5460823	-1.9420541	H	2.7374015	2.4188907	3.2343284
H	-2.2588886	0.8335453	-1.8458391	C	0.8054345	2.2714907	2.2831874
C	-1.7272186	1.6546523	1.3544969	H	0.5266725	3.3053657	2.4581704
H	-2.2983056	0.8558083	1.8511079	C	-0.0813155	1.4095107	1.6375104
H	-1.9434816	2.5631153	1.9333929	C	-1.4504345	1.9217067	1.2452994
C	4.0805794	-1.0648277	-0.0001641	H	-1.4273685	3.0190697	1.1837744
H	4.0895974	0.0378683	0.0095179	H	-2.1468995	1.6727287	2.0534664
H	4.6358624	-1.3972867	-0.8834301	C	1.8631695	-1.7361623	1.2627214
H	4.6264394	-1.4129287	0.8828449	H	0.9832335	-2.3710253	1.1852274
C	-0.9225266	-3.2415397	0.3772289	H	2.5128855	-2.1690703	2.0326144
H	-0.6914746	-3.2986637	1.4400329	H	-3.9474375	1.1937937	-0.8845686
H	-1.7827116	-3.8568887	0.1313999	H	4.4758365	-1.5975563	-0.8828536
H	-0.0702296	-3.5040657	-0.2481171	H	-0.6699115	-3.2695003	0.8979834
C	-3.6646666	2.1524853	-0.0184671	C	-2.7866265	-1.3806473	-1.4771596
H	-3.9235346	2.7769433	-0.8806331	H	-3.6824065	-1.8576473	-1.0823046
H	-4.2862836	1.2407553	-0.0714061	H	-3.0367105	-0.4322473	-1.9557966
H	-3.9563326	2.7011353	0.8826479	H	-2.2857165	-2.0367293	-2.1890616
[^{Me} LPd ^{IV} Me ₃] ⁺ TS_N ₃ N ₄ frequency=255.28 cm ⁻¹				[^{Me} LPd ^{IV} Me ₃] ⁺ N ₄			
Pd	1.2226444	-0.9581711	-0.0029253	Pd	1.4476788	0.6521076	0.0442664
N	-0.2612406	0.3804579	-1.3546543	N	-0.3331252	-0.1435094	-1.3763096
N	-2.3993746	-1.7154491	0.0077247	C	1.4370288	2.7158416	0.0479224
N	2.2027564	1.1746799	-0.0024963	H	0.9617058	3.0168076	0.9790834
C	2.4806344	-1.7025241	1.4274057	H	0.8493418	3.0237826	-0.8146756
H	1.9905624	-1.4609951	2.3736657	H	2.4464708	3.1190186	-0.0207276
H	3.4325534	-1.1802681	1.3271127	C	-1.5339382	0.4300506	-1.6089506
H	2.6371454	-2.7756671	1.3441127	C	-2.5632882	-0.2683694	-2.2495576
C	0.2470844	1.6159359	-1.5410763	H	-3.5083882	0.2292276	-2.4379406
C	-0.5270666	2.6821059	-2.0011513	C	-2.3734142	-1.5948514	-2.6207626
H	-0.0726096	3.6545029	-2.1590373	H	-3.1590952	-2.1489374	-3.1245326
C	-1.8833746	2.4780289	-2.2361343	C	-1.1719852	-2.2085194	-2.2842976
H	-2.5117206	3.2859449	-2.5975433	H	-1.0016482	-3.2586884	-2.4970596
C	-2.4195086	1.2219279	-1.9745043	C	-0.1820972	-1.4554514	-1.6497516
H	-3.4769116	1.0280419	-2.1167883	C	1.1205798	-2.1304724	-1.2712006
C	-1.5865526	0.1891739	-1.5291833	H	0.9745408	-3.2203774	-1.2667756
C	-2.1688636	-1.1923041	-1.3299453	H	1.8561848	-1.9215044	-2.0559096
H	-3.1266796	-1.2015451	-1.8731163	C	-1.7917502	1.8665546	-1.1921646
H	-1.5165476	-1.8874781	-1.8897673	H	-1.2133002	2.5207286	-1.8570666
C	1.7166824	1.8236989	-1.2494143	H	-2.8547512	2.0838066	-1.4021356
H	2.3007784	1.3944949	-2.0710613	N	-0.5379252	-0.3702664	1.3443054
H	1.9391574	2.9002729	-1.2305943	C	-1.7950582	0.0883606	1.4988484
C	-3.0949356	-2.9893331	-0.0260763	C	-2.8357142	-0.7462584	1.9293714
H	-4.1626486	-2.8852321	-0.2807413	H	-3.8319352	-0.3353554	2.0554964
H	-3.0284696	-3.4838501	0.9464797	C	-2.5869662	-2.0898374	2.1765764
C	3.6844624	1.2317949	-0.0086873	H	-3.3792552	-2.7491124	2.5169224
H	4.0380334	2.2713229	-0.0462553	C	-1.3070252	-2.5785574	1.9315404
H	4.0759504	0.6995709	-0.8765413	H	-1.0763772	-3.6312164	2.0574114
N	-0.2424796	0.3689619	1.3651457	C	-0.3181092	-1.6915454	1.5050474
C	0.2564244	1.6087179	1.5473547	C	1.0705998	-2.2205614	1.2286594
C	-0.5245676	2.6677149	2.0120307	H	1.0373608	-3.3191694	1.1890994
H	-0.0785876	3.6447169	2.1657047	H	1.7214308	-1.9542534	2.0689674
C	-1.8771866	2.4502419	2.2577197	C	-2.1289922	1.5514466	1.2571174
H	-2.5103536	3.2525769	2.6231447	H	-1.8825932	2.0922436	2.1799944
C	-2.4034246	1.1883329	2.0030187	H	-3.2271002	1.6280166	1.1518134
H	-3.4575396	0.9839609	2.1550757	C	2.9098758	0.9713086	-1.3520656

C	-1.5637596	0.1638029	1.5520097	H	2.5154498	1.6734486	-2.0862906
C	-2.1285556	-1.2250041	1.3538887	H	3.8237748	1.3564126	-0.9023786
H	-3.0647686	-1.2546191	1.9299337	H	3.0860978	-0.0007814	-1.8141906
H	-1.4419626	-1.9154291	1.8724687	C	2.8302088	0.8847286	1.5298734
C	1.7230354	1.8242359	1.2467437	H	2.2842758	0.5828676	2.4285654
H	2.3130754	1.3947369	2.0638567	H	3.6701558	0.2187376	1.3320144
H	1.9408534	2.9017389	1.2267527	H	3.1859058	1.9076426	1.6317894
H	-2.6428536	-3.6655161	-0.7657633	N	1.7315098	-1.6861614	0.0089314
H	4.0792564	0.7666819	0.8948407	N	-1.4280382	2.2387986	0.1776894
C	2.4504814	-1.7311591	-1.4451813	C	3.1354268	-2.1664464	0.0283974
H	3.0085994	-0.8823271	-1.8450963	H	3.1771418	-3.2613994	-0.0540736
C	3.1329784	-2.4814291	-1.0487543	H	3.6947538	-1.7344414	-0.8017546
H	1.8114814	-2.1625851	-2.2166393	H	3.6146148	-1.8744044	0.9629374
C	0.4727384	-2.8865561	0.0035347	C	-1.6099342	3.6872266	0.3367084
H	-0.0002936	-3.0453791	0.9721397	H	-1.0411302	4.2236916	-0.4264026
H	-0.2503746	-2.9489331	-0.8059353	H	-2.6666992	3.9941746	0.2509944
H	1.2658404	-3.6166241	-0.1467983	H	-1.2424782	4.0034176	1.3166314
^{Me} LPd ^{II} -O ₂ -DMPO adduct							
3-N ₂ (T)				3-N ₃ (S)			
Pd	0.5701518	-1.4440455	-0.1354409	Pd	0.7079048	-1.3464765	-0.0706196
N	1.4915278	0.1290245	1.3827121	N	1.8655438	0.1110975	1.4391134
N	4.1532338	-1.7348115	0.6472621	N	3.1739558	-2.1282135	0.0138514
N	0.2486178	2.4732755	-0.5952759	N	0.1290968	2.5859805	0.0389674
C	0.1773128	-2.9061665	-1.5177559	C	0.0514338	-2.6073945	-1.5499486
H	0.6152738	-3.8642265	-1.2194709	H	0.5402648	-3.5850455	-1.4772856
H	0.6229938	-2.5668645	-2.4590499	H	0.3125938	-2.1318925	-2.5027696
H	-0.9030292	-2.9994735	-1.6257549	H	-1.0302582	-2.7211435	-1.4763596
C	1.0279538	1.3874365	1.5527951	C	1.4310148	1.3411275	1.7920074
C	1.6250218	2.2572825	2.4756481	C	2.2435788	2.2088885	2.5374534
H	1.2072458	3.2492285	2.6135871	H	1.8469958	3.1699325	2.8478694
C	2.7324328	1.8409235	3.2044911	C	3.5440738	1.8376345	2.8540004
H	3.1985558	2.4986175	3.9329131	H	4.1903358	2.5008255	3.4220424
C	3.2356908	0.5640475	2.9739981	C	4.0097558	0.6043525	2.4058494
H	4.1075998	0.2011975	3.5088861	H	5.0296638	0.2867565	2.5989364
C	2.6003778	-0.2672875	2.0466451	C	3.1401808	-0.2370305	1.7079974
C	3.1870428	-1.6442535	1.7416591	C	3.6274408	-1.6213435	1.3096414
C	3.6986398	-1.9956595	2.6479781	H	4.7299018	-1.6387595	1.3909774
H	2.3703748	-2.3397425	1.5304261	H	3.2495518	-2.3235705	2.0624104
C	-0.1280782	1.8794545	0.6882921	C	0.0744738	1.8198705	1.2863914
H	-0.8372912	1.0711645	0.5025771	H	-0.6134312	0.9841355	1.1484344
H	-0.6619162	2.6519245	1.2566381	H	-0.3614662	2.4805555	2.0467754
C	1.0684858	3.6636735	-0.5455549	C	3.3019198	-3.5866275	-0.0435296
H	2.1358598	3.4964655	-0.3124649	H	4.3528318	-3.9247525	-0.0049096
H	1.0214138	4.1796665	-1.5126289	H	2.8497138	-3.9554955	-0.9665966
N	2.0708548	-0.1511645	-1.4247459	C	0.7878698	3.8715015	0.0936954
C	1.7704458	1.0292745	-2.0085979	H	1.8927668	3.8426265	0.1339534
C	2.7220378	1.7241205	-2.7669329	H	0.5080228	4.4608605	-0.7883246
H	2.4394378	2.6552775	-3.2474099	N	1.9872128	0.2029005	-1.3499726
C	4.0073128	1.2123785	-2.9001499	C	1.5589688	1.4412155	-1.6828306
H	4.7536368	1.7309045	-3.4955409	C	2.4053158	2.3479455	-2.3368236
C	4.3186958	0.0237165	-2.2471489	H	2.0164318	3.3159275	-2.6351616
H	5.3130898	-0.4060155	-2.3126599	C	3.7303198	2.0055795	-2.5775506
C	3.3318898	-0.6312125	-1.5037849	H	4.4034258	2.6987035	-3.0741706
C	3.6852368	-1.8993005	-0.7285609	C	4.1838718	0.7631365	-2.1443266
H	4.4842058	-2.4143035	-1.2794509	H	5.2199038	0.4675215	-2.2777546
H	2.8124008	-2.5588535	-0.7128659	C	3.2820108	-0.1176485	-1.5412596
C	0.3888478	1.6359645	-1.7841869	C	3.7710088	-1.5103985	-1.1696756
H	-0.3650782	0.8463425	-1.7429219	H	4.8742878	-1.4835375	-1.1040966
H	0.1651698	2.2695325	-2.6543719	H	3.5299668	-2.1668045	-2.0143236
H	0.6699348	4.3484615	0.2127651	C	0.1669168	1.8823405	-1.2436216
C	-0.3311162	-2.7178945	1.1969381	H	-0.5120042	1.0281005	-1.1841876
H	0.3397038	-3.5515605	1.4328031	H	-0.2241692	2.5751535	-2.0013336
H	-0.5338352	-2.1419905	2.1063941	H	2.7628278	-4.0325785	0.7950524
H	-1.2601722	-3.1109855	0.7824831	H	0.4413148	4.4188915	0.9787614
O	-1.4354092	-0.5031625	-0.6903389	C	-0.1133492	-2.7063095	1.2259844
O	-2.5786582	-1.3271565	-0.7829459	H	0.5149018	-3.6008065	1.3052134
C	-3.3877032	-1.1403965	0.3745581	H	-0.1691142	-2.2057975	2.1992864
C	-4.6210262	-2.0226245	0.1870831	H	-1.1136162	-2.9838935	0.8910464
H	-2.7907902	-1.3078855	1.2738851	O	-1.4659552	-0.4079805	-0.1083096
C	-5.3489892	0.3015505	-0.1231239	O	-2.5698952	-1.2285675	-0.2718906

C	-5.5746892	-1.1371765	-0.6448999	C	-3.4661512	-1.0419755	0.8457384
H	-5.0498382	-2.2564095	1.1671111	C	-4.6874382	-1.9170545	0.6233084
H	-4.3682342	-2.9622115	-0.3091849	H	-2.9036432	-1.1608955	1.7763014
H	-6.6207542	-1.4429425	-0.5532999	C	-5.1203862	0.3673985	-0.2599216
H	-5.2969502	-1.1986355	-1.7012579	C	-5.5110942	-1.1276045	-0.4262406
N	-3.9719912	0.2008785	0.4474751	H	-5.2284392	-2.0284725	1.5685314
O	-3.4274602	1.1767855	1.0631561	H	-4.4059242	-2.9138705	0.2756834
C	-6.3170272	0.6806275	1.0099571	H	-6.5871312	-1.2823585	-0.3020436
H	-5.9656322	1.5923555	1.4997921	H	-5.2437382	-1.4667625	-1.4305516
H	-7.3222462	0.8548355	0.6133391	N	-3.9694242	0.2979875	0.7043404
H	-6.3762142	-0.1108815	1.7641761	O	-3.1178882	1.2549195	0.7854184
C	-5.3610432	1.3667005	-1.2258289	C	-6.2236972	1.2016735	0.4106844
H	-6.3633572	1.4667725	-1.6557159	H	-5.8308892	2.1881555	0.6749254
H	-5.0590232	2.3324365	-0.8107819	H	-7.0753952	1.3331435	-0.2653096
H	-4.6614862	1.1019335	-2.0238189	H	-6.5797152	0.7195575	1.3271654
C	5.3765248	-0.9754165	0.8156191	C	-4.6656442	1.0219245	-1.5699976
H	5.7748338	-1.1481185	1.8223371	H	-5.5109922	1.1233865	-2.2590226
H	6.1258428	-1.3300825	0.0980261	H	-4.2508792	2.0112795	-1.3633306
H	5.2731288	0.1146795	0.6795151	H	-3.8878452	0.4180745	-2.0437586
3-N ₃ (T)				^{Me} L _{Pd} ^{II} -O ₂ complexes 2			
Pd	0.7050631	-1.4017731	-0.1606772	2_N ₂ (S)			
N	1.6667631	0.2150409	1.3810788	Pd	1.8698251	-0.8291930	-0.0000102
N	3.1063591	-2.1174891	0.2746108	N	0.1536401	-0.0224330	1.4141948
N	0.1603891	2.6222669	-0.3811182	N	0.1535951	-0.0224990	-1.4142142
C	0.2794331	-2.7954691	-1.6050752	N	0.7848001	2.9808870	-0.0000862
H	0.6580201	-3.7880391	-1.3430942	N	-1.3383249	-2.7106290	0.0000768
H	0.7708321	-2.4292891	-2.5137982	C	3.0327171	-1.7486990	1.4068798
H	-0.8010779	-2.8190101	-1.7406362	H	2.8688971	-2.8321720	1.3806468
C	1.2047671	1.4669819	1.5949518	H	2.7309921	-1.3575910	2.3858038
C	1.9222411	2.3729959	2.3915988	H	4.0796331	-1.5058010	1.2113828
H	1.5000921	3.3523749	2.5909778	C	3.0326791	-1.7487920	-1.4068742
C	3.1638861	2.0144849	2.9007128	H	4.0796021	-1.5058810	-1.2114312
C	3.7365241	2.7071029	3.5110948	H	2.7309191	-1.3577540	-2.3858152
C	3.6710341	0.7548789	2.5916898	H	2.8688591	-2.8322620	-1.3805552
H	4.6528111	0.4459539	2.9366508	C	-0.8234299	-0.9048140	1.7246078
C	2.8894791	-0.1221711	1.8365058	C	-1.9721689	-0.5074240	2.4156678
C	3.4056461	-1.5295621	1.5864858	H	-2.7248579	-1.2463120	2.6687438
H	4.4903471	-1.5481221	1.7954448	C	-2.1282709	0.8290110	2.7720188
H	2.9348321	-2.1839421	2.3297358	H	-3.0083869	1.1580590	3.3166518
C	-0.0664729	1.9156949	0.8837898	C	-1.1335749	1.7342310	2.4160388
H	-0.7215269	1.0649559	0.6849498	H	-1.2164929	2.7854320	2.6703918
H	-0.6085129	2.6036549	1.5439908	C	-0.0031939	1.2835910	1.7243798
C	3.2653151	-3.5756291	0.3288618	C	1.0509511	2.2813810	1.2641208
H	4.3099851	-3.8781671	0.5181028	H	1.1349071	3.0544350	2.0380758
H	2.9403401	-4.0126911	-0.6173692	H	2.0179381	1.7821200	1.1838828
C	0.8026981	3.9154669	-0.2970112	C	1.0509051	2.2813240	-1.2642702
H	1.8908161	3.8998499	-0.0983152	H	2.0178941	1.7820680	-1.1840522
H	0.6503021	4.4590359	-1.2378562	H	1.1348291	3.0543440	-2.0382642
N	2.1788571	0.1515869	-1.3674812	C	-0.0032559	1.2835120	-1.7244462
C	1.8319231	1.3843619	-1.7971862	C	-1.1336659	1.7341230	-2.4160772
C	2.7889971	2.2619399	-2.3289222	H	-1.2165959	2.7853140	-2.6704692
H	2.4701111	3.2254819	-2.7124702	C	-2.1283739	0.8288880	-2.7719812
C	4.1293361	1.8967549	-2.3412132	H	-3.0085129	1.1579120	-3.3165912
H	4.8858451	2.5673239	-2.7389532	C	-1.9722549	-0.5075330	-2.4155832
C	4.4855641	0.6605879	-1.8090882	H	-2.7249529	-1.2464320	-2.6685992
H	5.5242141	0.3481719	-1.7639832	C	-0.8234889	-0.9048930	-1.7245512
C	3.4812701	-0.1898491	-1.3404352	C	-0.6818729	-2.3504800	-1.2612112
C	3.8693811	-1.5763631	-0.8557642	H	-1.1088799	-2.9957060	-2.0381822
H	4.9543451	-1.5841351	-0.6476092	H	0.3814631	-2.5954760	-1.1711792
H	3.7099411	-2.2671601	-1.6923082	C	-0.6818259	-2.3504200	1.2613228
C	0.3938081	1.8505659	-1.6038282	H	0.3815101	-2.5954130	1.1712608
H	-0.2874879	0.9943569	-1.5999222	H	-1.1087969	-2.9956140	2.0383398
H	0.1298701	2.5002339	-2.4497572	C	-0.4118389	3.8081150	-0.0000832
H	2.6362111	-3.9831821	1.1222088	H	-1.3604799	3.2456290	-0.0000532
H	0.3321361	4.5010339	0.5020468	H	-0.4082289	4.4505460	-0.8876842
C	-0.2011179	-2.7459131	1.1054118	H	-0.4081969	4.4505880	0.8874878
H	0.4392571	-3.6164321	1.2790028	C	-2.7867329	-2.5696690	0.0001048
H	-0.3634689	-2.2075781	2.0454148	H	-3.1447659	-1.5272090	0.0000888
H	-1.1533439	-3.0681871	0.6843118	H	-3.1979889	-3.0629350	0.8876228
O	-1.2669279	-0.3965571	-0.5948742	H	-3.1980279	-3.0629760	-0.8873722

O	-2.4241419	-1.2346851	-0.7566672	O	3.5234691	0.7274900	-0.0001172
C	-3.2507359	-1.0809041	0.3766978	O	4.7774131	0.4180140	-0.0000372
C	-4.4854009	-1.9527361	0.1401718				
H	-2.6825909	-1.2697331	1.2923818				
C	-5.1969609	0.3801909	-0.1381672				
C	-5.4100659	-1.0455341	-0.7006042				
H	-4.9437409	-2.2017621	1.1032538				
H	-4.2250029	-2.8840631	-0.3678002				
H	-6.4600259	-1.3484991	-0.6500202				
H	-5.0976809	-1.0836171	-1.7481772				
N	-3.8457569	0.2600499	0.4843928				
O	-3.3389549	1.2104559	1.1689478				
C	-6.2090839	0.7396379	0.9625308				
H	-5.8721299	1.6369149	1.4878868				
H	-7.1965629	0.9294929	0.5296848				
H	-6.3035069	-0.0688641	1.6950098				
C	-5.1610759	1.4695839	-1.2169742				
H	-6.1452639	1.5868949	-1.6835242				
H	-4.8689299	2.4233929	-0.7682312				
H	-4.4314929	1.2173559	-1.9916782				
2_N ₂ (T)				2_N ₃ (S)			
Pd	1.2717990	-1.3876791	0.0000252	Pd	-1.6342419	-0.7236170	-0.0000301
N	0.0037510	-0.1887151	1.4025552	N	0.1676001	0.0018050	-1.3885421
N	0.0036870	-0.1887751	-1.4025048	N	-1.8301409	1.5969820	0.0000889
N	1.7639370	2.3147369	0.0000062	N	2.1108291	-2.3963400	0.0000779
N	-2.4115370	-2.0678831	0.0000322	C	-3.0784009	-1.0846030	1.3985749
C	2.3531340	-2.4253601	1.4070682	H	-3.9534349	-0.4472660	1.2440919
H	2.1731380	-3.5075841	1.3430192	H	-2.6325909	-0.8734450	2.3782479
H	2.0619860	-2.0954691	2.4148352	H	-3.3178969	-2.1450330	1.2871009
H	3.4328530	-2.2615081	1.2955122	C	1.3024451	-0.6712480	-1.6741131
C	2.3526910	-2.4257981	-1.4070268	C	2.3967001	-0.0258830	-2.2652951
H	3.4324170	-2.2615231	-1.2961388	H	3.2787301	-0.6019140	-2.5226611
H	2.0609160	-2.0965461	-2.4148218	C	2.3423781	1.3443170	-2.4988241
H	2.1730720	-3.5080391	-1.3422728	H	3.1851091	1.8640020	-2.9448431
C	-1.2287520	-0.6309401	1.7401502	C	1.1938851	2.0421470	-2.1311231
C	-2.1102860	0.1688649	2.4741422	H	1.1206471	3.1161960	-2.2656231
H	-3.0845680	-0.2233151	2.7456302	C	0.1217501	1.3355070	-1.5856491
C	-1.7227100	1.4522549	2.8490132	C	-1.1626289	2.0565520	-1.2429981
H	-2.3909460	2.0869919	3.4234682	H	-0.9782799	3.1390320	-1.1998991
C	-0.4611400	1.9050989	2.4736052	H	-1.8705029	1.8790970	-2.0595241
H	-0.1191210	2.8982289	2.7445592	C	1.4016821	-2.1329410	-1.2624091
C	0.3821180	1.0652399	1.7395902	H	0.3977691	-2.5542060	-1.1787341
C	1.7388130	1.5671839	1.2630832	H	1.9461771	-2.6705880	-2.0483171
H	2.1383230	2.2367329	2.0345942	C	-3.2207159	2.0993770	0.0000909
H	2.4150160	0.7130739	1.1677122	H	-3.2419069	3.1988560	0.0000439
C	1.7387730	1.5671159	-1.2630318	H	-3.7415279	1.7369550	0.8869659
H	2.4149400	0.7129809	-1.1676158	C	3.5209411	-2.0397810	0.0003959
H	2.1383050	2.2366089	-2.0345798	H	3.7254311	-0.9559080	0.0006449
C	0.3820660	1.0651819	-1.7395268	H	4.0018161	-2.4659240	0.8881739
C	-0.4611730	1.9050439	-2.4735578	N	0.1673781	0.0016710	1.3887859
H	-0.1191450	2.8981719	-2.7445038	C	1.3021711	-0.6715110	1.6742729
C	-1.7227350	1.4522029	-2.8489998	C	2.3966421	-0.0262000	2.2651009
H	-2.3909540	2.0869449	-3.4234708	H	3.2787201	-0.6022910	2.5221869
C	-2.1103220	0.1688109	-2.4741458	C	2.3425011	1.3440170	2.4985849
H	-3.0845980	-0.2233671	-2.7456588	H	3.1853981	1.8636490	2.9443539
C	-1.2288050	-0.6309941	-1.7401338	C	1.1940151	2.0419500	2.1310609
C	-1.6640830	-2.0104931	-1.2621138	H	1.1209341	3.1160220	2.2654579
H	-2.3123850	-2.4426131	-2.0342138	C	0.1217211	1.3353940	1.5857869
H	-0.7787950	-2.6456981	-1.1625028	C	-1.1625789	2.0565770	1.2431359
C	-1.6640310	-2.0104501	1.2621462	H	-0.9781119	3.1390340	1.1999619
H	-0.7787370	-2.6456441	1.1625092	H	-1.8704529	1.8792490	2.0596909
H	-2.3122960	-2.4425691	2.0342782	C	1.4013321	-2.1331550	1.2623899
C	0.9699550	3.5336599	-0.0000098	H	0.3974451	-2.5544110	1.1783889
H	-0.1205790	3.3697909	0.0000072	H	1.9456431	-2.6709330	2.0483319
H	1.2166350	4.1268749	-0.8875658	H	-3.7415469	1.7368760	-0.8867431
H	1.2166560	4.1269109	0.8875172	H	4.0021651	-2.4656150	-0.8873411
C	-3.6628100	-1.3261621	0.0000392	C	-3.0785839	-1.0838880	-1.3986331
H	-3.5445790	-0.2297821	0.0000212	H	-3.9534899	-0.4464460	-1.2438491
H	-4.2449220	-1.5976621	0.8876932	H	-2.6328309	-0.8724640	-2.3782761
H	-4.2449440	-1.5976871	-0.8875938	H	-3.3182659	-2.1443100	-1.2874801

O	4.7513040	0.2235199	-0.0004168	O	-1.3191879	-2.7942220	-0.0004531
O	5.3886700	-0.8099681	-0.0004068	O	-2.3526389	-3.6711210	-0.0006271
2_N ₃ (T)				2_N ₂ _(H ₂ O) ₃ (S)			
Pd	-1.6621037	0.0979847	0.0018998	Pd	0.9052078	-1.4606769	0.0619505
N	0.1572823	0.0718397	-1.3858152	N	-0.5100762	-0.0682259	-1.3238665
N	-0.6496467	2.5257797	0.0148458	N	-2.8024892	-2.3166439	-0.2192105
N	0.5424043	-2.9943313	-0.0137282	N	0.9951178	2.4914051	0.3316635
C	-3.1391847	0.2023897	1.4207518	C	1.2751438	-3.1705429	1.1275415
H	-3.5072497	1.2348667	1.5095818	H	0.6738258	-3.9983579	0.7401555
H	-2.7205037	-0.0940573	2.3934848	H	0.9988688	-2.9344729	2.1593975
H	-3.9851507	-0.4528073	1.1911408	H	2.3457238	-3.3631779	1.0503845
C	0.7719043	-1.0935843	-1.6854552	C	-0.2730352	1.2469941	-1.5113085
C	2.0368073	-1.1165773	-2.2845302	C	-1.1982362	2.0685521	-2.1632035
H	2.4870153	-2.0678563	-2.5461122	H	-0.9666572	3.1166741	-2.3178585
C	2.7040303	0.0817537	-2.5175092	C	-2.3954692	1.5216031	-2.6166935
C	3.6922983	0.0874147	-2.9675452	H	-3.1230712	2.1376191	-3.1366385
H	2.0890993	1.2745867	-2.1441462	C	-2.6396502	0.1692391	-2.3961385
H	2.5875963	2.2285667	-2.2816312	H	-3.5567562	-0.2972339	-2.7384555
C	0.8099093	1.2378107	-1.5861092	C	-1.6813622	-0.6020329	-1.7294235
C	0.1008393	2.5354917	-1.2424682	C	-1.9683372	-2.0605459	-1.3973475
H	0.8340843	3.3583177	-1.2758082	H	-2.4799672	-2.5101479	-2.2567225
H	-0.6265337	2.7245077	-2.0408302	H	-1.0166512	-2.5886469	-1.2623395
C	0.0885663	-2.3906193	-1.2753162	C	1.0283378	1.8181871	-0.9844355
H	-0.9861657	-2.2110883	-1.2009732	H	1.7817928	1.0309531	-0.9493255
C	0.2630253	-3.1357483	-2.0608422	H	1.3876478	2.5679361	-1.6977205
C	-1.6557817	3.5869257	0.0375588	C	-4.1615172	-1.8015159	-0.3044595
H	-1.2161687	4.5991767	0.0210048	H	-4.2422472	-0.7039169	-0.2422705
H	-2.2657907	3.4917667	0.9399858	H	-4.7589412	-2.2255159	0.5099035
C	1.9277903	-3.4399283	-0.0159342	C	0.1719068	3.7012091	0.3572665
H	2.6733423	-2.6274723	-0.0133372	H	-0.9062842	3.5074951	0.2673715
H	2.1097683	-4.0586993	0.8698668	H	0.3457648	4.2316861	1.2984865
N	0.1810223	0.0635197	1.3716638	N	-0.6867372	-0.2719149	1.4650365
C	0.7827743	-1.1092063	1.6716228	C	-0.4762742	1.0154361	1.8259435
C	2.0446573	-1.1475283	2.2753858	C	-1.4807922	1.7770431	2.4332975
H	2.4830733	-2.1042083	2.5372718	H	-1.2655062	2.7947521	2.7395125
C	2.7249483	0.0430867	2.5112108	C	-2.7358282	1.2149571	2.6464655
H	3.7113883	0.0374787	2.9652668	H	-3.5256672	1.7867741	3.1244065
C	2.1261063	1.2421717	2.1337798	C	-2.9552102	-0.0956909	2.2357905
H	2.6359433	2.1900647	2.2720038	H	-3.9181002	-0.5740199	2.3787235
C	0.8476073	1.2210737	1.5719198	C	-1.9143442	-0.8134599	1.6360895
C	0.1613913	2.5333927	1.2327418	C	-2.1830782	-2.2163989	1.1065965
H	0.9205953	3.3329967	1.2154748	H	-2.8577632	-2.7189299	1.8090885
H	-0.5169517	2.7619447	2.0630988	H	-1.2494832	-2.7799609	1.0842215
C	0.0902133	-2.3981523	1.2522508	C	0.8776438	1.6493381	1.5430595
H	-0.9831097	-2.2109053	1.1774508	H	1.6402928	0.8736261	1.4920995
C	0.2587613	-3.1505353	2.0321408	H	1.1265368	2.3029371	2.3859975
H	-2.3135867	3.4835097	-0.8298892	H	-4.6066282	-2.1142939	-1.2552575
H	2.1088683	-4.0527023	-0.9060522	H	0.4702948	4.3541991	-0.4689555
C	-3.1555277	0.2142877	-1.3989372	C	1.9945668	-2.3198099	-1.4299535
H	-3.5251947	1.2473507	-1.4734052	H	1.6192818	-3.3298999	-1.6210225
H	-2.7482587	-0.0728303	-2.3792102	H	1.8309698	-1.6856639	-2.3074725
H	-3.9983297	-0.4435813	-1.1653162	H	3.0518298	-2.3404819	-1.1578035
O	-3.0299507	-2.6880213	-0.0010502	O	2.7404798	-0.8149529	1.0100655
O	-4.2679217	-2.6496143	0.0085478	O	3.6128848	-1.6122109	1.5995535
2_N ₂ _(H ₂ O) ₃ (T)				2_N ₃ _(H ₂ O) ₃ (S)			
Pd	-0.2517544	-1.8854474	-0.0615637	Pd	-0.5665799	-1.4241202	-0.1472337
N	-0.7385764	-0.1225353	-1.3522327	N	0.5832721	0.0781538	1.3428773
N	-3.8696154	-1.0315113	-0.5177537	N	1.4115371	-2.4507042	0.1946243
N	1.6683136	1.2567137	0.5968423	N	-0.8076789	2.6888348	-0.3748057
C	0.1435386	-3.4176883	1.2507223	C	-1.1638149	-2.7677492	-1.5656567
H	-0.4161204	-4.3278194	0.9935653	H	-1.2631699	-3.7803522	-1.1679157

H	-0.1472324	-3.1189703	2.2681073	H	-0.3894449	-2.7380712	-2.3400167
H	1.2094976	-3.6803074	1.2669443	H	-2.1103989	-2.3458832	-1.9094987
C	0.1369466	0.9051277	-1.4286907	C	0.4073931	1.4081048	1.4795253
C	-0.1934194	2.0975037	-2.0777247	C	1.3859251	2.2121798	2.0778873
H	0.5425676	2.8915016	-2.1415637	H	1.1968601	3.2717168	2.2097123
C	-1.4606884	2.2424927	-2.6363617	C	2.5864211	1.6411848	2.4875553
H	-1.7372044	3.1583097	-3.1500997	H	3.3611951	2.2495018	2.9442223
C	-2.3640374	1.1894697	-2.5259817	C	2.7834641	0.2761608	2.2870013
H	-3.3609754	1.2614307	-2.9473747	H	3.7148151	-0.2061432	2.5638363
C	-1.9801584	0.0161197	-1.8684007	C	1.7563861	-0.4736482	1.7152003
C	-2.9763764	-1.1209133	-1.6792397	C	1.9118761	-1.9605622	1.5098953
H	-3.6161764	-1.1563553	-2.5691207	H	2.9615521	-2.2517142	1.6408173
H	-2.4259604	-2.0644393	-1.6155967	H	1.3249721	-2.4761692	2.2772143
C	1.4984596	0.7346647	-0.7800867	C	-0.8734759	2.0125618	0.9424253
H	1.7459326	-0.3295283	-0.7626187	H	-1.6377209	1.2448638	0.8870993
H	2.2412846	1.2520387	-1.3962627	H	-1.2168209	2.7720238	1.6530023
C	-4.7470014	0.1291747	-0.5149407	C	1.3593771	-3.9321732	0.2473973
H	-4.2371074	1.0891387	-0.3291557	H	2.3636141	-4.3447822	0.4130793
H	-5.5110834	0.0038637	0.2601673	H	0.9652931	-4.3187802	-0.6917377
C	1.4194186	2.6968617	0.7173923	C	-0.0183969	3.9203268	-0.3634657
H	0.3652936	2.9723057	0.5833923	H	1.0619331	3.7590268	-0.2345917
H	1.7396806	3.0318657	1.7085483	H	-0.1695979	4.4525738	-1.3078887
N	-1.1508994	-0.4363703	1.3903573	N	0.9213011	-0.0722162	-1.3932337
C	-0.3765294	0.5211927	1.9487473	C	0.7623841	1.2202678	-1.7516997
C	-0.9306614	1.5561197	2.7066753	C	1.8480921	1.9753188	-2.2137637
H	-0.2791344	2.2961697	3.1585043	H	1.6859461	2.9972618	-2.5379627
C	-2.3116164	1.6163247	2.8743193	C	3.1198111	1.4107168	-2.2360927
H	-2.7631984	2.4084947	3.4639493	H	3.9745341	1.9868328	-2.5774357
C	-3.1010004	0.6402277	2.2738213	C	3.2819441	0.1000268	-1.7920197
H	-4.1803254	0.6501157	2.3811343	H	4.2600851	-0.3679242	-1.7598787
C	-2.4945804	-0.3735543	1.5245013	C	2.1556601	-0.6145672	-1.3853627
C	-3.3467434	-1.4086624	0.8013053	C	2.2821771	-2.0576642	-0.9512867
H	-4.2145994	-1.6290523	1.4345463	H	3.3296211	-2.2876842	-0.7192097
H	-2.7621144	-2.3265304	0.6867583	H	1.9861681	-2.6888372	-1.7948167
C	1.1221916	0.4549787	1.7163413	C	-0.6098519	1.8554188	-1.5879537
H	1.4083376	-0.5860223	1.5490943	H	-1.3715359	1.0788238	-1.5820357
H	1.6290046	0.8118267	2.6193553	H	-0.7816419	2.5220328	-2.4396687
H	-5.2520934	0.2043617	-1.4842917	H	0.7098601	-4.2460892	1.0644903
H	2.0126546	3.2234917	-0.0362267	H	-0.3641719	4.5615628	0.4538763
C	0.5181726	-3.1090173	-1.5221407	C	-1.6949859	-2.5116192	1.1640903
H	-0.1257984	-3.9839044	-1.6890997	H	-1.3240369	-3.5366212	1.2289473
H	0.5852696	-2.5554784	-2.4698817	H	-1.5705039	-1.9979602	2.1233193
H	1.5209596	-3.4814153	-1.2761077	H	-2.7358809	-2.4745952	0.8365693
O	3.7300826	-1.8707213	-0.1318577	O	-2.2608949	-0.3304152	-0.4581447
O	3.5923596	-1.9109313	1.0730383	O	-3.0787609	-0.5828582	-1.5574427
H	3.3651406	1.1688087	0.7993673	H	-2.6663479	2.9810428	-0.3121687
O	4.3710766	1.1728257	0.7797503	O	-3.6252229	3.0483118	-0.0796207
H	4.6336446	2.0556077	1.0758843	H	-3.6447859	3.7308338	0.6056383
O	4.8392026	0.6635446	-1.8955427	O	-3.9802569	0.5686728	1.3956343
H	4.1929406	-0.0408403	-2.0405987	H	-3.3415779	0.0622998	0.8424093
H	4.6478976	0.9705927	-0.9812467	H	-4.0259109	1.4057708	0.8914503
O	6.4485116	-0.7219943	0.1021873	O	-4.9297599	-1.7856002	-0.0789617
H	5.8240996	-0.2275143	0.6569433	H	-4.2718969	-1.4067762	-0.7339587
H	6.1703026	-0.4257393	-0.7804987	H	-4.9583469	-1.0601262	0.5657323
2_N3_(H2O)3 (T)				2_N2_(H) (S)			
Pd	0.0958903	-1.6230734	-0.0227551	Pd	1.8182523	-0.8169545	0.0266107
N	0.7625433	0.1852036	1.3676648	N	0.0895733	-0.0563655	1.4383247
N	2.5469813	-1.7875124	0.1650049	N	0.0955663	-0.0477725	-1.3993243
N	-1.6419807	1.9551466	-0.2657041	N	0.7646353	2.9404925	0.0372887
C	-0.1083637	-3.1068254	-1.4241652	N	-1.5352347	-2.6584505	-0.0016783
H	0.0367183	-4.1120224	-1.0172572	C	2.8401823	-1.8247875	1.4796827
H	0.6464693	-2.9138874	-2.1961622	H	2.4421443	-2.8407275	1.4200717
H	-1.1158247	-3.0026864	-1.8364302	H	2.5812323	-1.3302485	2.4170267
C	0.0440433	1.3138986	1.5392389	H	3.9051113	-1.7736695	1.2627557
C	0.6143193	2.4609836	2.1039188	C	2.8924523	-1.6814345	-1.4706803
H	-0.0004637	3.3384896	2.2702428	H	3.8634103	-1.9847055	-1.0784683
C	1.9668113	2.4607246	2.4301969	H	2.9832613	-0.9294715	-2.2575543
H	2.4330243	3.3434546	2.8572378	H	2.2936103	-2.5333605	-1.7994663
C	2.7171763	1.3138736	2.1805308	C	-0.9098757	-0.9172065	1.7481697
H	3.7812313	1.2824666	2.3896168	C	-2.0362257	-0.4957535	2.4617087

C	2.0815533	0.1886506	1.6541669	H	-2.8049547	-1.2181305	2.7134317
C	2.8633783	-1.0883244	1.4247858	C	-2.1541237	0.8375985	2.8390237
H	3.9398833	-0.8738184	1.4957958	H	-3.0174597	1.1814815	3.4006797
H	2.6154433	-1.7783254	2.2388139	C	-1.1425527	1.7202645	2.4779777
C	-1.3924187	1.3257406	1.0524729	H	-1.1951147	2.7707125	2.7424567
H	-1.7683777	0.3052466	1.0077768	C	-0.0330267	1.2519845	1.7662897
H	-2.0037637	1.8776786	1.7740388	C	1.0220643	2.2501425	1.3067527
C	3.0261133	-3.1775954	0.2184819	H	1.0903313	3.0278155	2.0764997
H	4.1248313	-3.2280824	0.2640529	H	1.9975633	1.7679875	1.2505897
H	2.6837253	-3.7116594	-0.6701232	C	1.0440803	2.2481225	-1.2266223
C	-1.3422027	3.3874516	-0.3133261	H	2.0097383	1.7493735	-1.1397773
H	-0.2700917	3.6205566	-0.2576032	H	1.1443673	3.0244505	-1.9943433
H	-1.7337557	3.8017786	-1.2473872	C	-0.0139737	1.2647455	-1.7125023
N	0.9522623	0.0899056	-1.3963832	C	-1.1126127	1.7479135	-2.4311213
C	0.2496253	1.1762816	-1.7804362	H	-1.1562127	2.8012785	-2.6853213
C	0.8776453	2.2719916	-2.3829652	C	-2.1264867	0.8752335	-2.8106033
H	0.2805723	3.1116746	-2.7207532	H	-2.9826837	1.2313935	-3.3755633
C	2.2624033	2.2736036	-2.5222032	C	-2.0210257	-0.4635945	-2.4481063
H	2.7717073	3.1190576	-2.9746062	H	-2.7919807	-1.1781335	-2.7150453
C	2.9852743	1.1807536	-2.0507772	C	-0.9032057	-0.9000065	-1.7300713
H	4.0683873	1.1559496	-2.1086531	C	-0.8542827	-2.3508435	-1.2602173
C	2.2971313	0.0984696	-1.4996901	H	-1.3264777	-2.9628325	-2.0373603
C	3.0619803	-1.1298214	-1.0507502	H	0.1825713	-2.6910705	-1.1737923
H	4.1251373	-0.8722694	-0.9359962	C	-0.8566057	-2.3625765	1.2614827
H	2.9969913	-1.8669654	-1.8584942	H	0.1786943	-2.7033985	1.1730187
C	-1.2375937	1.2086766	-1.4799292	H	-1.3303707	-2.9830665	2.0308627
H	-1.6139207	0.1909406	-1.3890242	C	-0.4266817	3.7764455	0.0281307
H	-1.7532947	1.6901426	-2.3175451	H	-1.3782267	3.2196675	0.0225907
H	2.6174663	-3.6734434	1.1006509	H	-0.4118367	4.4175605	-0.8599683
H	-1.8437437	3.8841366	0.5232868	H	-0.4233167	4.4192875	0.9151227
C	-0.4177317	-3.0290884	1.3836198	C	-2.9737617	-2.4395995	-0.0031473
H	0.4153893	-3.7159994	1.5639069	H	-3.2740397	-1.3792845	0.0011537
H	-0.6427057	-2.4734234	2.3028248	H	-3.4119857	-2.9139845	0.8813207
H	-1.3014997	-3.5921184	1.0740728	H	-3.4086737	-2.9056225	-0.8936993
O	-2.4552667	-1.5524774	-0.1270601	O	3.3110153	0.5275485	0.1687687
O	-3.0296447	-1.8068404	-1.2714122	O	4.6499273	0.1225515	0.0597757
H	-3.4142617	1.9228816	-0.2492941	H	4.8132233	0.1689985	-0.9031313
O	-4.3999877	1.8957776	-0.1059161				
H	-4.5782737	2.6687246	0.4480799				
O	-4.4176597	-0.3630644	1.5206568				
H	-3.7080577	-0.8587274	1.0653589				
H	-4.4855997	0.4529286	0.9751588				
O	-5.7815127	-1.9102784	-0.4252701				
H	-4.9124667	-1.9118784	-0.8682401				
H	-5.5716457	-1.3930314	0.3746579				
2_N ₂ _(H) (T)				2_N ₃ _(H) (S)			
Pd	1.2758680	-1.2807855	-0.0103004	Pd	1.5289628	0.6518118	0.0452278
N	-0.0710290	-0.1450045	1.4088646	N	-0.1973072	-0.0106732	-1.3788922
N	-0.0838870	-0.1455165	-1.4074564	N	1.8524788	-1.4942842	-0.0011822
N	1.5196650	2.4724055	-0.0101314	N	-2.2708972	2.2518328	0.0525438
N	-2.3259650	-2.2317595	0.0136466	C	2.9350638	0.9158808	1.5045748
C	2.3549820	-2.2873525	1.4063826	H	3.9109798	0.5948758	1.1399208
H	2.0081710	-3.3255275	1.3923466	H	2.6008078	0.3038618	2.3456928
H	2.1415920	-1.8207265	2.3719296	H	2.9326538	1.9766428	1.7449668
H	3.4179700	-2.2249665	1.1655816	C	-1.3587912	0.6169278	-1.6609612
C	2.3404060	-2.2638845	-1.4529034	C	-2.4054152	-0.0666032	-2.2928892
H	3.3709050	-1.9049735	-1.4054774	H	-3.3134892	0.4707188	-2.5426892
H	1.8840870	-2.0230635	-2.4165514	C	-2.2744662	-1.4218932	-2.5767382
H	2.2895530	-3.3383305	-1.2539404	H	-3.0825362	-1.9673232	-3.0543632
C	-1.2714290	-0.6754295	1.7328496	C	-1.0955252	-2.0734302	-2.2193862
C	-2.2237440	0.0721865	2.4305606	H	-0.9608302	-3.1354142	-2.3935812
H	-3.1709890	-0.3857165	2.6938696	C	-0.0756302	-1.3312052	-1.6283272
C	-1.9370900	1.3887295	2.7817976	C	1.2398578	-1.9802892	-1.2814352
H	-2.6613450	1.9839015	3.3297656	H	1.1290488	-3.0686122	-1.2351852
C	-0.7052730	1.9278865	2.4212786	H	1.9563648	-1.7553082	-2.0766372
H	-0.4428770	2.9482695	2.6784296	C	-1.5450112	2.0588668	-1.2107582
C	0.2123970	1.1391715	1.7217656	H	-0.5708922	2.5397498	-1.1200612
C	1.5362610	1.7283715	1.2523976	H	-2.1167842	2.5800318	-1.9875852
H	1.8877260	2.4203815	2.0263226	C	3.2701078	-1.9587392	0.0260688
H	2.2752250	0.9246165	1.1648926	H	3.2932308	-3.0536552	-0.0154312

C	1.5244100	1.7283145	-1.2726784	H	3.7475608	-1.6263452	0.9460938
H	2.2663630	0.9261435	-1.1931234	C	-3.6592502	1.8141828	0.0381048
H	1.8664310	2.4209005	-2.0502834	H	-3.7985522	0.7205488	0.0187968
C	0.1963930	1.1372665	-1.7280704	H	-4.1675152	2.1962358	0.9302638
C	-0.7284490	1.9222155	-2.4222144	N	-0.2260732	-0.0774122	1.3957998
H	-0.4696480	2.9418515	-2.6859164	C	-1.3806992	0.5509318	1.7066148
C	-1.9628900	1.3800485	-2.7694504	C	-2.4349172	-0.1468002	2.3087598
H	-2.6926040	1.9723175	-3.3133104	H	-3.3353072	0.3910928	2.5839538
C	-2.2453180	0.0645335	-2.4108054	C	-2.3228852	-1.5157852	2.5285768
H	-3.1943230	-0.3952345	-2.6642464	H	-3.1374732	-2.0716302	2.9825278
C	-1.2862300	-0.6792565	-1.7183314	C	-1.1546042	-2.1655022	2.1368118
C	-1.6009210	-2.0963905	-1.2519214	H	-1.0336782	-3.2363562	2.2593248
H	-2.2128890	-2.5751465	-2.0248384	C	-0.1245132	-1.4096772	1.5809878
H	-0.6657300	-2.6648805	-1.1702054	C	1.1826958	-2.0621612	1.2153498
C	-1.5936140	-2.0931525	1.2747786	H	1.0474778	-3.1404812	1.0802938
H	-0.6619180	-2.6658325	1.1913566	H	1.8779618	-1.9188212	2.0472818
H	-2.2036410	-2.5659995	2.0528136	C	-1.5566522	2.0104788	1.3148158
C	0.6959890	3.6725905	-0.0066684	H	-0.5812412	2.4937478	1.2550668
H	-0.3894510	3.4799255	-0.0014184	H	-2.1367612	2.5004958	2.1054758
H	0.9241170	4.2700865	-0.8959384	H	3.8118078	-1.5588782	-0.8295712
H	0.9325940	4.2710055	0.8797736	H	-4.1589032	2.2270978	-0.8450862
C	-3.6723160	-1.6777125	0.0167896	C	2.9136158	1.0820438	-1.3954152
H	-3.7100300	-0.5760865	0.0157926	H	3.2757508	0.1557218	-1.8399742
H	-4.2055220	-2.0290325	0.9066646	H	2.3622748	1.6712468	-2.1318932
H	-4.2102940	-2.0307035	-0.8695574	H	3.7267768	1.6580318	-0.9551912
O	4.3989160	0.2402825	0.0090516	O	1.1516138	2.6356038	0.0934338
O	5.1769920	-0.8353565	0.0247626	O	2.2772238	3.5257308	0.1176868
H	6.1024010	-0.4955785	0.0412736	H	2.4522848	3.6528878	-0.8317832
2_N ₃ _(H) (T)				2_N ₂ _(H ₂ O) (S)			
Pd	1.4758787	0.2567960	-0.0343350	Pd	1.6752614	-0.9705163	-0.5044738
N	-0.2477353	0.1045360	1.3785720	N	0.3306044	0.1586777	1.2476672
N	0.6962327	2.4212810	-0.0152330	N	-0.3652876	-0.2270893	-1.4716268
N	-0.7091413	-2.9321620	-0.0189410	N	0.5919174	2.9229787	-0.7205538
C	2.9370987	0.4155300	-1.4658360	N	-1.4548946	-2.6536493	0.6363892
H	3.6150877	1.2499110	-1.2689360	C	3.0787634	-2.0542533	0.5226062
H	2.4433347	0.5589970	-2.4329500	H	2.7497214	-3.0918403	0.6415542
C	3.5035647	-0.5222550	-1.4761150	H	3.1793984	-1.5618863	1.4928352
C	-0.8713253	-1.0515400	1.6821730	H	4.0234574	-1.9970293	-0.0198958
C	-2.1154483	-1.0408690	2.3224840	C	2.3237964	-2.0092473	-2.1360688
H	-2.5873573	-1.9803910	2.5875240	H	3.3623264	-1.7540533	-2.3529218
C	-2.7352263	0.1759980	2.5942300	H	1.6718774	-1.6929943	-2.9567148
H	-3.7070833	0.2027410	3.0773990	H	2.2197104	-3.0831243	-1.9547078
C	-2.1009113	1.3610760	2.2229020	C	-0.5526266	-0.6365533	1.8951942
H	-2.5635623	2.3269850	2.3950130	C	-1.5369246	-0.1063283	2.7352622
C	-0.8474233	1.2876570	1.6196250	H	-2.2078856	-0.7770543	3.2606322
C	-0.0737823	2.5328520	1.2520630	C	-1.6352356	1.2735327	2.8878252
H	-0.7452763	3.3990470	1.2091940	H	-2.3848786	1.7067927	3.5434112
H	0.6560457	2.7193670	2.0460970	C	-0.7534246	2.0857057	2.1823912
C	-0.2202903	-2.3547900	1.2382610	H	-0.7958536	3.1658147	2.2697772
H	0.8599577	-2.2066110	1.1462300	C	0.2160594	1.5032707	1.3577432
H	-0.3912753	-3.1032670	2.0210810	C	1.1388734	2.3937987	0.5347252
C	1.7785947	3.4274880	-0.0379280	H	1.4039734	3.2584227	1.1546812
H	1.3610117	4.4430270	-0.0352090	H	2.0543564	1.8535737	0.3040032
H	2.3814797	3.2891730	-0.9359190	C	0.5481584	2.0350727	-1.8878118
C	-2.1055413	-3.3431340	-0.0065410	H	1.5032444	1.5127057	-1.9572998
H	-2.8276643	-2.5101660	-0.0006920	H	0.4532364	2.6768877	-2.7720748
H	-2.3097753	-3.9536960	-0.8928020	C	-0.5901396	1.0247377	-1.9245098
N	-0.2901813	0.1112410	-1.3923720	C	-1.8573086	1.4180607	-2.3704108
C	-0.9114223	-1.0443330	-1.7033860	H	-1.9987346	2.4235617	-2.7514678
C	-2.1645663	-1.0348830	-2.3246160	C	-2.9127696	0.5127507	-2.3234918
H	-2.6334653	-1.9748790	-2.5935940	H	-3.9018116	0.7968837	-2.6706038
C	-2.7967903	0.1810980	-2.5711720	C	-2.6757956	-0.7650463	-1.8240508
H	-3.7753193	0.2076650	-3.0406360	H	-3.4702786	-1.5015293	-1.7695538
C	-2.1655933	1.3647770	-2.1913410	C	-1.3897636	-1.1071763	-1.3953698
H	-2.6368533	2.3298190	-2.3437490	C	-1.1346816	-2.4819163	-0.7841118
C	-0.9027693	1.2925670	-1.6065080	H	-1.7363686	-3.2123643	-1.3376258
C	-0.1356863	2.5431840	-1.2416130	H	-0.0811326	-2.7494913	-0.9257108
H	-0.8218053	3.3937580	-1.1470260	C	-0.5142276	-2.1376313	1.6390162
H	0.5498127	2.7648450	-2.0655220	H	0.4960074	-2.4266613	1.3342362
C	-0.2486873	-2.3484260	-1.2835130	H	-0.7397526	-2.6508763	2.5810062

H	0.8329797	-2.1963180	-1.2182880	C	-0.5546946	3.8061017	-0.5782488
H	-0.4365543	-3.0925540	-2.0663480	H	-1.4909866	3.3040187	-0.2829618
H	2.4107547	3.2972870	0.8406170	H	-0.7386996	4.3166287	-1.5302608
H	-2.2942553	-3.9535970	0.8831820	H	-0.3335556	4.5657127	0.1797242
C	2.9857417	0.4053700	1.3483230	C	-2.8625056	-2.4926873	0.9699552
H	3.6224547	1.2747490	1.1677040	H	-3.2314336	-1.4555483	0.9117982
H	2.5298927	0.4766660	2.3415550	H	-3.0350376	-2.8501963	1.9908672
H	3.5981487	-0.5011450	1.2866950	H	-3.4672196	-3.0996643	0.2871852
O	2.8099067	-3.2485390	-0.0797800	O	3.2339704	0.4612087	-0.8996278
O	4.0739087	-2.8354550	-0.0534540	O	4.3858944	0.4141357	-0.2698408
H	4.2508827	-2.5864780	0.8834300	H	3.8336534	0.7112267	1.3956532
				O	3.4066834	0.8022137	2.2808702
				H	2.5229614	0.4419337	2.1349872
2_N ₂ _(H ₂ O) (T)				2_N ₃ _(H ₂ O) (S)			
Pd	-0.6866936	-1.7213849	-0.0268301	Pd	1.6133018	0.0881039	0.3909009
N	0.3036224	-0.2485049	-1.3958421	N	-0.1166892	0.2586859	-1.2358261
N	0.2570004	-0.2571939	1.3996699	N	1.3992058	-2.0520301	-0.3645491
N	-2.0254866	1.7853281	-0.0285721	N	-1.7579962	2.4353649	0.7686129
N	3.0504914	-1.5850509	0.0373009	C	2.9385388	-0.2671871	1.9027369
C	-1.4138776	-2.9902849	-1.4651711	H	3.5561418	-1.1412491	1.6841899
H	-1.0026996	-4.0031839	-1.3522781	H	2.3305938	-0.4415031	2.7965659
H	-1.1313906	-2.6191509	-2.4607871	H	3.5402108	0.6359439	2.0140199
H	-2.5066906	-3.0647429	-1.4219101	C	-1.0648612	1.2136729	-1.3403501
C	-1.4933206	-3.0099659	1.3527999	C	-2.1726632	1.0398629	-2.1805261
H	-2.4627056	-3.4133189	1.0410459	H	-2.8952672	1.8425349	-2.2777891
H	-1.6289516	-2.4868939	2.3105329	C	-2.3396262	-0.1626251	-2.8597561
H	-0.8157216	-3.8582879	1.5297089	H	-3.2006382	-0.3209871	-3.5022401
C	1.6122964	-0.4000899	-1.7012681	C	-1.3923672	-1.1696721	-2.6846921
C	2.3159454	0.5946101	-2.3876071	H	-1.4987892	-2.1344021	-3.1693111
H	3.3596184	0.4335561	-2.6351371	C	-0.2870982	-0.9175731	-1.8722281
C	1.6655134	1.7712551	-2.7479621	C	0.7974768	-1.9591421	-1.7225021
H	2.1929464	2.5535841	-3.2855371	H	0.4177188	-2.9413021	-2.0333921
C	0.3241504	1.9248121	-2.4080261	H	1.6113038	-1.6928631	-2.4045041
H	-0.2213856	2.8243641	-2.6716731	C	-0.9492002	2.4503149	-0.4606571
C	-0.3321856	0.8995541	-1.7210281	H	0.0945408	2.5902229	-0.1784071
C	-1.7804706	1.0632531	-1.2924131	H	-1.2823252	3.3150929	-1.0479301
H	-2.3114426	1.6206091	-2.0721431	C	2.6623798	-2.8185091	-0.4750021
H	-2.2364476	0.0734641	-1.2080621	H	2.4651268	-3.8376871	-0.8347091
C	-1.8162956	1.0646621	1.2425419	H	3.1435038	-2.8774441	0.5013289
H	-2.2734316	0.0776001	1.1476819	C	-3.1973162	2.4006009	0.5627449
H	-2.3659876	1.6251301	2.0068179	H	-3.5906492	1.4417919	0.1854419
C	-0.3814876	0.8940341	1.7089769	H	-3.7043232	2.6147409	1.5104379
C	0.2604134	1.9170091	2.4127749	N	-0.4418872	-0.6195781	1.3761459
H	-0.2885736	2.8186561	2.6617279	C	-1.4709252	0.1413239	1.8053449
C	1.5915544	1.7583771	2.7879689	C	-2.7247942	-0.4244251	2.0733709
H	2.1077874	2.5382081	3.3398589	H	-3.5198712	0.2043329	2.4588489
C	2.2464834	0.5796631	2.4431989	C	-2.9365432	-1.7768741	1.8276879
H	3.2829134	0.4148391	2.7170049	H	-3.9052632	-2.2296301	2.0168119
C	1.5575924	-0.4117609	1.7371359	C	-1.8875352	-2.5374101	1.3147689
C	2.2833394	-1.6731309	1.2858859	H	-2.0163112	-3.5881121	1.0777409
H	2.9929414	-1.9510639	2.0745059	C	-0.6507832	-1.9261261	1.1111649
H	1.5546444	-2.4818679	1.1806959	C	0.5252848	-2.7400381	0.6242479
C	2.3264834	-1.6633379	-1.2371291	H	0.1728328	-3.6952481	0.2134439
H	1.5956794	-2.4741879	-1.1638581	H	1.1552158	-2.9684031	1.4902449
H	3.0624634	-1.9327739	-2.0041791	C	-1.2717332	1.6459179	1.9109919
C	-1.5534546	3.1690961	-0.0227171	H	-0.2123102	1.8642419	2.0474159
H	-0.4581056	3.2665811	-0.0069341	H	-1.8174092	1.9981229	2.7946939
H	-1.9538776	3.6793591	0.8589099	H	3.3341318	-2.3194411	-1.1731961
H	-1.9279086	3.6779761	-0.9164911	H	-3.4771192	3.1770979	-0.1581711
C	4.1438404	-0.6243679	0.0591979	C	3.2520268	0.4804839	-0.7593501
H	3.8264954	0.4316921	0.0560689	H	4.0314838	-0.2716431	-0.6114901
H	4.7818324	-0.7824209	-0.8172851	H	2.9094608	0.4693419	-1.7992911
H	4.7496554	-0.7863379	0.9575609	H	3.5731738	1.4720559	-0.4399081
O	-4.0091946	-1.3027969	0.0701289	O	1.6270508	1.9983569	1.1254199
O	-4.6076756	-2.3638099	0.0276579	O	2.7475608	2.8000659	1.0345289
H	-5.0534076	0.9184071	0.0701489	H	2.4179778	3.3843209	-0.4525701
O	-4.8461036	1.8561671	-0.0280271	O	2.1419808	3.6920319	-1.3736641
H	-3.8607306	1.8740601	-0.0386411	H	1.3240728	4.1764799	-1.2078381
2_N ₃ _(H ₂ O) (T)				2_N ₂ _(H ₃ O) (S)			
N	-0.3010278	0.2067494	-1.3791671	Pd	-0.8048278	-1.9084770	-0.0041222

N	-2.5516378	-1.0487696	-0.0001501	N	0.2064552	-0.1490380	-1.4161752
N	2.6598702	1.1017664	0.0000349	N	0.2423512	-0.2081400	1.3811708
C	-0.1087028	-3.1516926	1.3998079	N	-2.1794638	1.8218610	0.0384428
H	-1.0640618	-3.6902596	1.3811059	N	3.0228372	-1.4943720	-0.0718362
H	0.0155652	-2.6873256	2.3876099	C	-1.2672838	-3.3068880	-1.4123422
H	0.7132252	-3.8485166	1.2167979	H	-0.4775238	-4.0626560	-1.4461632
C	0.7396722	1.0168604	-1.6665921	H	-1.3099938	-2.7397840	-2.3476822
C	0.5456262	2.2710434	-2.2566851	H	-2.2340698	-3.7519900	-1.1788722
H	1.4057412	2.8799884	-2.5116991	C	-0.8481448	-3.4426510	1.3488818
C	-0.7497998	2.7218314	-2.4911401	H	-1.8030388	-3.9620010	1.2701888
H	-0.9247618	3.6966874	-2.9363171	H	-0.7423968	-2.9567020	2.3232228
C	-1.8190728	1.9074844	-2.1254731	H	-0.0088188	-4.1132320	1.1471498
H	-2.8450838	2.2325714	-2.2620891	C	1.5150282	-0.2774250	-1.7187672
C	-1.5606998	0.6496634	-1.5781521	C	2.2240752	0.7590260	-2.3407222
C	-2.7131688	-0.2761066	-1.2402221	H	3.2656952	0.6083790	-2.6014212
H	-3.6490378	0.3041204	-1.2323201	C	1.5825752	1.9595340	-2.6218472
H	-2.7933568	-1.0036166	-2.0561981	H	2.1125492	2.7719460	-3.1090472
C	2.1311302	0.5593374	-1.2682041	C	0.2418972	2.0973980	-2.2699202
H	2.1457122	-0.5295106	-1.2049951	H	-0.3000948	3.0139190	-2.4741222
H	2.8364852	0.8637344	-2.0492131	C	-0.4135848	1.0254470	-1.6603342
C	-3.4430128	-2.2140926	-0.0001421	C	-1.8676538	1.1410720	-1.2874512
H	-4.5069108	-1.9262906	-0.0001871	H	-2.3924528	1.7465660	-2.0294992
H	-3.2467078	-2.8222836	0.8857959	H	-2.3439638	0.1603540	-1.2408902
C	2.8717632	2.5464604	0.0003549	C	-1.8447778	1.0653380	1.3171478
H	1.9438952	3.1374384	0.0003349	H	-2.2960078	0.0783190	1.2144058
H	3.4491562	2.8237614	0.8882029	H	-2.3732398	1.6145390	2.0995468
N	-0.3010398	0.2064634	1.3789739	C	-0.3848118	0.9523910	1.6717988
C	0.7397842	1.0162884	1.6666979	C	0.2689872	2.0099890	2.3072748
C	0.5459272	2.2702704	2.2573079	H	-0.2800018	2.9115160	2.5549418
H	1.4061372	2.8789874	2.5125319	C	1.6183612	1.8783460	2.6261158
C	-0.7494278	2.7211344	2.4919559	H	2.1481942	2.6809810	3.1293828
H	-0.9242798	3.6958204	2.9375489	C	2.2686262	0.6968190	2.2902318
C	-1.8188368	1.9070994	2.1259379	H	3.3183112	0.5526250	2.5210158
H	-2.8447878	2.2323304	2.2626669	C	1.5595742	-0.3307800	1.6542908
C	-1.5606698	0.6494834	1.5780929	C	2.3056812	-1.5822870	1.2025968
C	-2.7132848	-0.2759976	1.2398259	H	3.0501972	-1.8203020	1.9706758
H	-3.6489818	0.3045094	1.2316699	H	1.6152452	-2.4259720	1.1477808
H	-2.7939278	-1.0034296	2.0558219	C	2.2491732	-1.5511730	-1.3151152
C	2.1311492	0.5586874	1.2679859	H	1.5362352	-2.3788760	-1.2429102
H	2.1453882	-0.5300976	1.2038699	H	2.9539752	-1.7987490	-2.1173202
H	2.8366282	0.8623704	2.0491549	C	-1.7819848	3.2586380	0.0728328
H	-3.2466698	-2.8223456	-0.8860321	H	-0.6966628	3.3456840	0.0519188
H	3.4494642	2.8241214	-0.8871831	H	-2.1743268	3.7026860	0.9879998
C	-0.1083038	-3.1517276	-1.3999941	H	-2.2129448	3.7545590	-0.7973932
H	-1.0633448	-3.6908546	-1.3811541	C	4.1461082	-0.5670290	-0.0832692
H	0.0155392	-2.6873496	-2.3878601	H	3.8622552	0.4977390	-0.0530842
H	0.7140212	-3.8481416	-1.2171631	H	4.7374342	-0.7281330	-0.9909652
O	2.5461202	-2.4562716	0.0004819	H	4.7852322	-0.7660940	0.7836258
O	2.7651722	-3.7102616	0.0005409	O	-2.8560168	-1.8562880	0.4564238
H	4.2391492	-1.4181326	-0.0012101	O	-3.6192108	-1.4344550	-0.5613442
O	4.8773602	-0.6865076	-0.0010541	H	-3.2355928	1.7548060	0.0516498
H	4.2776632	0.0881444	-0.0003691	O	-4.6905008	0.9104830	0.0275548
				H	-4.3246238	-0.0057200	-0.1709622
				H	-5.0730408	0.8482560	0.9153088
2_N2_(H2O) (T)				2_N3_(H3O) (S)			
Pd	-0.5332954	-1.7986123	0.0650847	Pd	1.1726529	-1.3174619	-0.0903710
N	0.3691826	-0.3340723	-1.3948773	N	0.0670919	0.2791471	1.3995330
N	0.4142406	-0.2436743	1.3887657	N	2.6552689	0.3736101	0.1072230
N	-2.0431794	1.6323857	-0.0284213	N	-2.8673111	-0.6338619	-0.1222850
N	3.2079366	-1.5068353	-0.0054753	C	2.2052769	-2.2103369	-1.6109840
C	-1.3249134	-3.1332643	-1.2746043	H	3.2785949	-2.1758269	-1.4272450
H	-0.6467274	-3.9884233	-1.4089933	H	1.9350459	-1.6313609	-2.4987380
H	-1.4456624	-2.6441743	-2.2513043	H	1.8425979	-3.2354909	-1.6767680
H	-2.2997044	-3.5201793	-0.9595683	C	-1.2587931	0.4538021	1.5717900
C	-1.2603924	-3.0284923	1.5337027	C	-1.7822001	1.6449971	2.0843340
H	-2.3548904	-3.0816033	1.5047817	H	-2.8504261	1.7346821	2.2472390
H	-0.9574134	-2.6383873	2.5158487	C	-0.9192601	2.6996651	2.3700960
H	-0.8685394	-4.0497483	1.4361037	H	-1.3030341	3.6376971	2.7584460
C	1.6714456	-0.4464583	-1.7332493	C	0.4429999	2.5344041	2.1327580
C	2.3163826	0.5551877	-2.4690163	H	1.1480559	3.3384341	2.3137680

H	3.3574796	0.4252237	-2.7436293	C	0.8990739	1.3074351	1.6488050
C	1.6153306	1.6960517	-2.8434923	C	2.3652989	1.0704601	1.3948690
H	2.0971886	2.4795927	-3.4197043	H	2.9151369	2.0182171	1.4329940
C	0.2783216	1.8132587	-2.4683863	H	2.7524759	0.4271951	2.1912000
H	-0.3071184	2.6840467	-2.7414493	C	-2.1466721	-0.7042909	1.2180310
C	-0.3104674	0.7840107	-1.7325283	H	-1.5771791	-1.6443069	1.2011360
C	-1.7563534	0.8680797	-1.3139963	H	-2.9529951	-0.7910709	1.9506250
H	-2.3364234	1.3929577	-2.0768793	C	4.0822399	-0.0387439	0.1385630
H	-2.1600104	-0.1358653	-1.1792803	H	4.7278379	0.8391401	0.2683910
C	-1.7179024	0.9445307	1.2918857	H	4.3456119	-0.5334509	-0.7952930
H	-2.1185134	-0.0679333	1.2200467	C	-3.9520581	0.3864421	-0.1627790
H	-2.2806344	1.5085037	2.0383297	H	-3.5280211	1.3891601	-0.1176730
C	-0.2607074	0.8918887	1.6741807	H	-4.5117091	0.2614861	-1.0908220
C	0.3446266	1.9675477	2.3246907	N	0.1701439	0.3876881	-1.3444600
H	-0.2367844	2.8521977	2.5588327	C	-1.1388651	0.5242011	-1.6365230
C	1.6927616	1.8782777	2.6664217	C	-1.6464311	1.7159981	-2.1593090
H	2.1877916	2.6986347	3.1764427	H	-2.6943191	1.7829061	-2.4289680
C	2.3877306	0.7171557	2.3461127	C	-0.7922871	2.8057201	-2.3171520
H	3.4367086	0.6068107	2.5986467	H	-1.1665841	3.7458331	-2.7096340
C	1.7257016	-0.3319153	1.6963037	C	0.5432029	2.6764591	-1.9453310
C	2.4908746	-1.5796983	1.2722347	H	1.2322049	3.5106901	-2.0211330
H	3.2381356	-1.7926153	2.0455087	C	0.9932979	1.4454791	-1.4652470
H	1.7942936	-2.4223823	1.2276127	C	2.4425499	1.2413581	-1.0892320
C	2.4462466	-1.6657423	-1.2489953	H	2.9336739	2.2103061	-0.9397740
H	1.7482376	-2.4979383	-1.1200313	H	2.9401679	0.7441961	-1.9277760
H	3.1650486	-1.9377823	-2.0309483	C	-2.0201061	-0.6720249	-1.3846070
C	-1.5843364	3.0550357	-0.0779483	H	-1.4098501	-1.5748559	-1.3000590
H	-0.4964204	3.0954517	-0.0924733	H	-2.7406711	-0.7848259	-2.1973140
H	-1.9667064	3.5662677	0.8058067	H	4.2434589	-0.7273149	0.9684000
H	-1.9897274	3.5127327	-0.9803723	H	-4.6099701	0.2242201	0.6915390
C	4.2628706	-0.5051193	-0.0585933	C	2.1416769	-2.5563529	1.2094730
H	3.9032156	0.5369967	-0.0874693	H	3.0478259	-2.9876929	0.7797910
H	4.8728786	-0.6709203	-0.9532103	H	2.3829689	-1.9244079	2.0699950
H	4.9073656	-0.6100793	0.8208607	H	1.4008399	-3.3161939	1.4586920
O	-3.9428644	-1.3743063	-0.0167453	O	-0.1214801	-2.8507549	-0.4439670
O	-4.4901534	-2.4492183	-0.1836723	O	-0.8071201	-3.3221799	0.6978900
H	-3.0918534	1.6766667	-0.0075933	H	-2.2354721	-3.3427139	0.2110330
O	-4.7852264	1.7481707	0.0260387	O	-3.2269271	-3.2438239	-0.1025970
H	-5.2322924	0.9310747	-0.2437223	H	-3.2888291	-1.6173629	-0.1455800
H	-5.1328234	1.9366997	0.9123897	H	-3.7587031	-3.5743199	0.6350090
2_N ₃ _(H ₂ O) (T)				2_N ₂ _(H ₂ O) ₂ (S)			
Pd	0.2196997	-1.6538184	-0.0178580	Pd	-0.5534761	-1.8572691	-0.1631374
N	0.3653227	0.2354056	1.3603920	N	0.2336729	-0.1474711	1.3171816
N	2.6153317	-1.0046374	0.0069070	N	3.1619289	-1.5349291	0.3410386
N	-2.6490533	1.0084776	-0.0421550	N	-1.8694541	1.8756209	-0.4320934
C	0.2723827	-3.1500304	-1.4135820	C	-0.6355471	-3.4246531	-1.4765034
H	1.2237987	-3.6907094	-1.3673860	H	0.0990269	-4.1759661	-1.1672804
H	0.1727977	-2.6731384	-2.3970700	H	-0.3736951	-3.0179391	-2.4590454
H	-0.5626823	-3.8331304	-1.2412710	H	-1.6432651	-3.8421061	-1.4907024
C	-0.6877003	1.0351656	1.6231430	C	-0.4273601	1.0153079	1.4946546
C	-0.5296073	2.2954226	2.2032930	C	0.1354209	2.0650269	2.2290326
H	-1.4013153	2.8939546	2.4421020	H	-0.4324821	2.9763739	2.3807446
C	0.7585217	2.7646566	2.4536470	C	1.4127859	1.9185369	2.7623236
H	0.9119337	3.7454656	2.8924610	H	1.8654109	2.7178129	3.3415846
C	1.8438497	1.9623856	2.1142930	C	2.0982149	0.7269739	2.5416016
H	2.8625747	2.3033446	2.2647960	H	3.0958019	0.5724359	2.9382726
C	1.6130797	0.6947866	1.5732590	C	1.4853219	-0.2908831	1.8039576
C	2.7739767	-0.2223164	1.2470820	C	2.2481759	-1.5727701	1.4877606
H	3.7049317	0.3629316	1.2297600	H	2.8495699	-1.8341271	2.3663986
H	2.8590967	-0.9434354	2.0675200	H	1.5298889	-2.3841511	1.3233876
C	-2.0526103	0.5053326	1.2688840	C	-1.7979641	1.1625319	0.8630176
H	-2.0289993	-0.5809614	1.2021120	H	-2.2633581	0.1848409	0.7337496
H	-2.7808343	0.7997546	2.0271930	H	-2.4308921	1.7298539	1.5536576
C	3.5236147	-2.1616834	0.0164720	C	4.2780439	-0.6112381	0.4807336
H	4.5800487	-1.8523764	0.0219870	H	4.0017019	0.4542589	0.4222186
H	3.3407357	-2.7732414	-0.8692070	H	5.0115619	-0.8091361	-0.3083414
C	-2.9227413	2.4772866	-0.0376610	C	-1.4331041	3.2704019	-0.3753094
H	-1.9846083	3.0299116	-0.0260220	H	-0.3519531	3.3932979	-0.2182464
H	-3.4917483	2.7218236	-0.9351330	H	-1.7001241	3.7678389	-1.3129654
N	0.3928117	0.2411546	-1.3888250	N	0.6152699	-0.2123951	-1.4738934

C	-0.6516543	1.0473836	-1.6650760	C	0.0512109	0.9571049	-1.8545714
C	-0.4775473	2.3127686	-2.2295810	C	0.8162739	1.9892259	-2.4086614
H	-1.3418733	2.9174576	-2.4790160	H	0.3255689	2.9023199	-2.7276574
C	0.8167647	2.7789016	-2.4515490	C	2.1904979	1.8248759	-2.5533264
H	0.9821617	3.7631136	-2.8782100	H	2.7998209	2.6098879	-2.9912084
C	1.8923207	1.9684936	-2.1003680	C	2.7663329	0.6330709	-2.1252994
H	2.9150547	2.3060316	-2.2298100	H	3.8336489	0.4628459	-2.2152794
C	1.6461327	0.6974536	-1.5748370	C	1.9552099	-0.3648861	-1.5735804
C	2.7954717	-0.2280884	-1.2339800	C	2.5983769	-1.6270781	-1.0115794
H	3.7313357	0.3488886	-1.2075420	H	3.4219549	-1.9105231	-1.6773794
H	2.8830827	-0.9532654	-2.0506190	H	1.8702889	-2.4430111	-1.0206704
C	-2.0262813	0.5184346	-1.3458820	C	-1.4425671	1.1566559	-1.6518364
H	-2.0066173	-0.5689104	-1.2907690	H	-1.9503531	0.1950669	-1.6677084
H	-2.7371513	0.8229866	-2.1162910	H	-1.8199351	1.7455409	-2.4947264
H	3.3298577	-2.7676354	0.9036470	H	4.7631409	-0.7750181	1.4493246
C	-3.5086633	2.7134396	0.8511460	H	-1.9554301	3.7747519	0.4438896
C	0.2523307	-3.1524574	1.3758460	C	-1.2967011	-3.1235051	1.2465076
H	1.2019367	-3.6967774	1.3374180	H	-0.5184101	-3.8031411	1.6108956
H	0.1458087	-2.6773514	2.3595280	H	-1.6468941	-2.4846131	2.0647256
H	-0.5836893	-3.8319384	1.1940130	H	-2.1380621	-3.6703681	0.8154256
O	-2.3876363	-2.3951714	-0.0406370	O	-2.6041591	-1.5752911	-0.8835764
O	-2.6097213	-3.6670644	-0.0356710	O	-3.5755701	-2.4053411	-0.6047984
H	-3.9265593	-1.5367104	-0.0538660	H	-3.6845921	1.7921299	-0.4872374
O	-4.6255743	-0.8378684	-0.0606360	O	-4.6567551	1.6445589	-0.3558314
H	-3.5757383	0.5042236	-0.0499650	H	-4.9203921	2.3569319	0.2431116
H	-5.0761623	-0.9241204	0.7935760	O	-4.5306101	-0.6818211	1.3767796
				H	-4.2388651	-1.3877331	0.7624596
				H	-4.6221501	0.0912839	0.7880136
2_N ₂ _(H ₂ O) ₂ (T)				2_N ₃ _(H ₂ O) ₂ (S)			
Pd	0.2720346	-1.9644936	0.3711041	Pd	0.6284108	-1.5932766	-0.2268975
N	0.4638006	0.0282724	1.3756741	N	0.2219548	0.1925554	1.3011345
N	3.7003006	-0.4426176	0.5430991	N	2.7191718	-0.7476126	0.1775955
N	-2.1783504	0.6542814	-0.6443959	N	-2.6077092	0.9351894	-0.4216365
C	0.1381146	-3.7142556	-0.6974769	C	1.1834928	-2.9547936	-1.6435405
H	0.8673386	-4.4599216	-0.3512559	H	2.1624538	-3.3800176	-1.4116365
H	0.3380436	-3.5159266	-1.7602489	H	1.2183178	-2.4098156	-2.5931655
H	-0.8589634	-4.1677496	-0.6201679	H	0.4000738	-3.7140426	-1.6518185
C	-0.5775034	0.8901744	1.3381911	C	-0.9299732	0.8681474	1.4908455
C	-0.4454594	2.2109694	1.7760861	C	-0.9542352	2.0660564	2.2160215
H	-1.3087014	2.8673344	1.7563871	H	-1.9014372	2.5643734	2.3903675
C	0.7900766	2.6580444	2.2367241	C	0.2371168	2.6050394	2.6915445
H	0.9141366	3.6791144	2.5849521	H	0.2398038	3.5392364	3.2448985
C	1.8619686	1.7701124	2.2437451	C	1.4294858	1.9337734	2.4296825
H	2.8411296	2.0778354	2.5946951	H	2.3842048	2.3323984	2.7559845
C	1.6739416	0.4576574	1.7983021	C	1.3811898	0.7230384	1.7382465
C	2.8492966	-0.5093056	1.7374441	C	2.6468688	-0.0654426	1.4967975
H	3.4956986	-0.3050506	2.5995801	H	3.5220978	0.5828524	1.6355555
H	2.4684686	-1.5310456	1.8275201	H	2.7000588	-0.8521066	2.2569155
C	-1.9025654	0.3951604	0.7875011	C	-2.1916782	0.3156994	0.8600715
H	-1.9768494	-0.6821996	0.9538361	H	-2.0906502	-0.7571536	0.6936325
H	-2.7108974	0.8913824	1.3332871	H	-3.0223772	0.4764864	1.5554075
C	4.3631706	0.8367864	0.3402801	C	3.8043418	-1.7533506	0.2402155
H	3.6926446	1.6576794	0.0362021	H	4.7688928	-1.2703656	0.4498875
H	5.1294696	0.7291024	-0.4353399	H	3.8740858	-2.2797376	-0.7114645
C	-2.2126904	2.0788134	-0.9876279	C	-2.9931652	2.3415864	-0.3120565
H	-1.2291814	2.5663494	-0.9393519	H	-2.1551952	3.0215404	-0.1012305
H	-2.5991604	2.1898264	-2.0056679	H	-3.4610182	2.6593944	-1.2492475
N	0.8844756	-0.6173546	-1.3077249	N	0.6210738	0.4784484	-1.4236375
C	-0.0610714	0.0930004	-1.9631649	C	-0.4501622	1.2324494	-1.7489235
C	0.2831186	1.0846644	-2.8858609	C	-0.3023802	2.5736514	-2.1261265
H	-0.5008294	1.6209164	-3.4095069	H	-1.1755192	3.1425214	-2.4254665
C	1.6270506	1.3623624	-3.1210919	C	0.9589628	3.1600144	-2.0976595
H	1.9172646	2.1254434	-3.8370679	H	1.0911588	4.2018404	-2.3736665
C	2.5913116	0.6408544	-2.4231399	C	2.0472768	2.3927384	-1.6870265
H	3.6488866	0.8245324	-2.5797749	H	3.0423258	2.8188154	-1.6153115
C	2.1922886	-0.3409696	-1.5102279	C	1.8407658	1.0518164	-1.3636195
C	3.2309506	-1.0925436	-0.6868139	C	3.0037508	0.1767734	-0.9541925
H	4.1132406	-1.2449256	-1.3200759	H	3.8756058	0.8010974	-0.7192915
H	2.8260856	-2.0733906	-0.4195359	H	3.2710498	-0.4532616	-1.8087595
C	-1.5193164	-0.1995616	-1.6539969	C	-1.8314692	0.6072374	-1.6399045

H	-1.6082794	-1.2367966	-1.3223539	H	-1.7445102	-0.4779556	-1.6942635
H	-2.0972884	-0.0819486	-2.5773489	H	-2.4340612	0.9542804	-2.4863635
H	4.8575796	1.1401204	1.2697911	H	3.5897968	-2.4726766	1.0307715
H	-2.8933864	2.5849774	-0.2976109	H	-3.7265222	2.4486114	0.4939515
C	-0.2747564	-3.0774576	2.0094381	C	0.7285248	-3.1297546	1.1082005
H	0.4651306	-3.8574876	2.2377261	H	1.6765288	-3.6689336	1.0336285
H	-0.3593564	-2.4260926	2.8912771	H	0.6265898	-2.6816056	2.1028605
H	-1.2428034	-3.5754126	1.8653511	H	-0.1290962	-3.7585676	0.8561695
O	-3.5960484	-2.7579356	-0.6074419	O	-1.2794512	-2.1662866	-0.7095235
O	-3.6817984	-2.6049316	0.5932051	O	-1.6986032	-3.4753236	-0.6329655
H	-3.8949894	0.2488654	-0.7028969	H	-4.0972252	-0.0989006	-0.5539235
O	-4.8845764	0.1649354	-0.6083139	O	-4.8641282	-0.7221436	-0.4725835
H	-5.2366114	0.5182684	-1.4374439	H	-5.4387302	-0.2925746	0.1760635
O	-4.8308084	2.2036494	1.2735381	O	-3.5493992	-2.7730406	1.2027635
H	-4.8516404	1.7426184	2.1227781	H	-2.8513072	-3.1204206	0.5858195
H	-4.9631354	1.4852674	0.6152101	H	-4.0154262	-2.1285036	0.6408715
2_N ₂ _(H ₂ O) ₂ (T)				3			
Pd	0.4122490	-1.6478273	-0.1128758	Pd	1.5266934	0.6806984	-0.0030624
N	0.3925400	0.1708417	1.3708042	N	-0.2178336	-0.0751036	-1.4057204
N	2.8234650	-0.9795493	0.2079592	N	1.8631744	-1.5019266	0.0250216
N	-2.4030130	1.0811877	-0.3203448	N	-2.3392656	2.1217964	-0.0218964
C	0.6875560	-3.0512993	-1.5777958	C	2.9375434	1.0490714	1.4396356
H	1.5451280	-3.6974923	-1.3548848	H	3.8799334	0.5784884	1.1602906
H	0.8797290	-2.5200943	-2.5196548	H	2.5246864	0.6233234	2.3566266
H	-0.2187950	-3.6560413	-1.6653358	H	3.0355204	2.1294114	1.5003316
C	-0.6850400	0.9626527	1.5553892	C	-1.3814856	0.5279164	-1.7346304
C	-0.5798480	2.1978227	2.2057242	C	-2.3849266	-0.1818046	-2.4098044
H	-1.4726230	2.7886207	2.3778952	H	-3.2911076	0.3350884	-2.7064674
C	0.6715130	2.6542147	2.6069932	C	-2.2166936	-1.5339276	-2.6832394
H	0.7787420	3.6146927	3.1019412	H	-2.9884256	-2.0954936	-3.2004054
C	1.7877580	1.8639937	2.3438412	C	-1.0451496	-2.1623276	-2.2630044
H	2.7857180	2.1949487	2.6113442	H	-0.8874256	-3.2227976	-2.4294084
C	1.6134270	0.6221197	1.7307752	C	-0.0674486	-1.3952376	-1.6335474
C	2.8095160	-0.2795333	1.5009472	C	1.2517214	-2.0206606	-1.2415134
H	3.7325190	0.3017327	1.6520542	H	1.1483364	-3.1114396	-1.1750994
H	2.7862790	-1.0533583	2.2768032	H	1.9778564	-1.8158696	-2.0353384
C	-2.0148640	0.5052047	0.9889612	C	-1.6243276	1.9669414	-1.2876694
H	-2.0211420	-0.5785993	0.8963602	H	-0.6718166	2.4913234	-1.2103684
H	-2.8116650	0.7771787	1.6882172	H	-2.2237916	2.4629444	-2.0609394
C	3.7457840	-2.1205203	0.2542982	C	3.2780504	-1.9728156	0.0573276
H	4.7918630	-1.8054923	0.3997142	H	3.3086254	-3.0693066	0.0713226
C	3.6776670	-2.6824383	-0.6799888	H	3.7749064	-1.5947936	0.9494356
C	-2.5818080	2.5351157	-0.3063178	C	-3.7286806	1.7016484	-0.0055084
H	-1.6460660	3.0993747	-0.1949038	H	-4.2252966	2.1306014	0.8716056
H	-3.0588520	2.8435717	-1.2417798	H	-4.2358326	2.0944644	-0.8935864
N	0.7122980	0.2738207	-1.3737578	N	-0.2275886	-0.0435936	1.3944906
C	-0.3126850	1.0570077	-1.7731808	C	-1.3732336	0.5897404	1.7332486
C	-0.0886410	2.3187357	-2.3349468	C	-2.3696876	-0.0813456	2.4555976
H	-0.9307470	2.9052247	-2.6849238	H	-3.2584166	0.4605854	2.7601876
C	1.2112610	2.8092557	-2.4154798	C	-2.2185876	-1.4282666	2.7640376
H	1.4073300	3.7918507	-2.8339588	H	-2.9863496	-1.9604186	3.3169796
C	2.2537260	2.0259287	-1.9280708	C	-1.0706146	-2.0896596	2.3317576
H	3.2778570	2.3837837	-1.9404578	H	-0.9272166	-3.1478586	2.5241546
C	1.9721850	0.7561007	-1.4200278	C	-0.0950786	-1.3581126	1.6571866
C	3.1128710	-0.1312443	-0.9569018	C	1.2045714	-2.0231986	1.2661816
H	4.0038410	0.4928977	-0.7862878	H	1.0600764	-3.1072926	1.1727536
H	3.3540570	-0.8055483	-1.7863908	H	1.9226694	-1.8683126	2.0782346
C	-1.7287130	0.5642257	-1.5336678	C	-1.6067866	2.0141244	1.2405746
H	-1.7328760	-0.5250073	-1.4782118	H	-0.6508246	2.5266304	1.1300396
H	-2.3522770	0.8683527	-2.3816558	H	-2.1927716	2.5440804	2.0010196
H	3.4659290	-2.7829743	1.0765362	H	3.8116584	-1.6211806	-0.8243394
H	-3.2425010	2.8035207	0.5237602	H	-3.8912956	0.6097354	0.0180186
C	0.3000700	-3.2256873	1.1933802	C	2.9493254	1.1167094	-1.4108434
H	1.3072980	-3.5856443	1.4367492	H	3.6277814	0.2742254	-1.5420004
H	-0.1800860	-2.8626183	2.1118382	H	2.3857424	1.3146094	-2.3246284
O	-0.2941480	-4.0434903	0.7775012	H	3.4865444	1.9998624	-1.0708554
H	-2.1325510	-2.4823373	-0.3740848	O	1.0753094	2.6347064	-0.0528954
O	-2.3280890	-3.6687413	-0.8061458	O	2.1188214	3.5872434	0.1279066
H	-4.0960520	0.5641447	-0.4735658	H	2.2484094	3.9167754	-0.7771924
O	-5.0587790	0.3103567	-0.4679828				

H	-5.4824260	1.0178907	0.0378262			
O	-4.4029840	-1.7749163	1.3044642			
H	-3.6784090	-2.1254063	0.7617742			
H	-4.7644940	-1.0705093	0.7297312			
3+H				Int4		
Pd	-1.3706378	0.6465484	-0.0135205	Pd	2.9517688	1.2470306
N	0.2173722	-0.2807776	1.3856495	N	3.9059198	-0.5739154
N	-2.0611428	-1.3440226	-0.0101875	N	5.0326078	1.8799686
N	2.7347862	1.5621684	0.0071375	N	2.0571168	-2.7191164
C	-2.7368268	1.1784534	-1.4778775	C	2.4365428	2.7689946
H	-3.7419508	1.1360724	-1.0628925	H	1.8954138	3.5453516
H	-2.5864108	0.4765584	-2.2975225	H	3.3398948	3.1684016
H	-2.4765848	2.1935604	-1.7692585	H	1.8100168	2.2861256
C	1.4855752	0.1127094	1.6222325	C	3.4818888	-1.8546364
C	2.4110902	-0.7610506	2.2060295	C	4.3150008	-2.8484724
H	3.4203232	-0.4130076	2.3970685	H	3.9331058	-3.8579874
C	2.0322112	-2.0599446	2.5227075	C	5.6153728	-2.5383864
H	2.7354672	-2.7453276	2.9847875	H	6.2709508	-3.2995524
C	0.7359192	-2.4776926	2.2118385	C	6.0685738	-1.2314424
H	0.4140982	-3.4942636	2.4123845	H	7.0854548	-0.9525794
C	-0.1364838	-1.5614706	1.6356865	C	5.1821198	-0.2806474
C	-1.5524738	-1.9432576	1.2862075	C	5.6058958	1.1588436
H	-1.6606508	-3.0311696	1.2229735	H	6.6990718	1.2383566
H	-2.2321438	-1.5929076	2.0687475	H	5.2661538	1.7085466
C	1.9175572	1.5123174	1.2284285	C	2.1054648	-2.2142394
H	1.0348662	2.1688714	1.1752455	H	1.4709658	-1.3363014
H	2.5360352	1.9010934	2.0414655	H	1.6757408	-2.9886614
C	-3.5432778	-1.5931836	-0.0632775	C	5.2957138	3.3379536
H	-3.7093328	-2.6736096	-0.1244425	H	6.3763258	3.5193316
H	-3.9747188	-1.1193206	-0.9421755	H	4.8309398	3.9267696
C	3.6594962	2.7089214	0.0213825	C	2.6419278	-4.0295344
H	4.3243242	2.6544364	-0.8432935	H	2.2931598	-4.4153894
H	3.1424092	3.6830674	0.0019085	H	2.2939448	-4.7207504
N	0.2751542	-0.3069876	-1.3764225	N	3.9426098	-0.1244084
C	1.5478812	0.0748334	-1.6147235	C	3.4908958	-1.2740584
C	2.4804892	-0.8124886	-2.1641585	C	4.3177038	-2.0413684
H	3.4905382	-0.4674736	-2.3560395	H	3.9190078	-2.9356174
C	2.1089282	-2.1214716	-2.4447635	C	5.6392978	-1.6621504
H	2.8170112	-2.8186666	-2.8809275	H	6.2927658	-2.2508754
C	0.8128212	-2.5296536	-2.1279565	C	6.1177378	-0.5223484
H	0.4939142	-3.5529276	-2.2966805	H	7.1515208	-0.2111924
C	-0.0674868	-1.5976686	-1.5877285	C	5.2351768	0.2227756
C	-1.4806088	-1.9966646	-1.2484635	C	5.6978028	1.5116256
H	-1.5530608	-3.0815176	-1.1187975	H	6.7836578	1.4930306
H	-2.1461528	-1.7293696	-2.0744245	H	5.4926128	2.3325276
C	2.0062952	1.4753534	-1.2529715	C	2.1016908	-1.7717544
H	1.1382942	2.1672514	-1.3089715	H	1.4731668	-0.9185564
H	2.6805182	1.8121984	-2.0443055	H	1.6684028	-2.2725354
H	-4.0271038	-1.2213116	0.8366615	H	4.9022178	3.6513606
H	4.2782262	2.6673014	0.9201125	H	3.7447528	-4.0557244
C	-2.7065518	1.2348084	1.4534445	C	2.4005378	2.4302426
H	-3.5868518	0.5994084	1.4471495	H	2.7512608	1.8773586
H	-2.1310238	1.1473804	2.3754415	H	1.3175948	2.4907466
H	-2.9580108	2.2631834	1.2041215	H	2.8633878	3.4108376
O	-0.7814568	2.7949364	0.0629775	O	0.9550358	0.8181876
O	-1.8573388	3.7585954	-0.1234385	O	0.3466138	0.5308106
H	-1.6542418	4.3954964	0.5895665	H	-0.2432912	-0.2379934
H	-0.1990768	3.0016814	-0.6961375	Pd	-2.8164912	-0.9485164
				N	-4.1974512	0.8766426
				N	-3.7065022	-0.8491184
				N	-6.5489212	-1.4697844
				N	-1.6113452	1.8654926
				C	-2.1841492	-0.8810734
				H	-1.0973132	-0.8538684
				H	-2.6179292	0.0108386
				H	-2.5587332	-1.7731924
				C	-1.6485892	-2.6262384
				H	-2.3490612	-3.4669644
				H	-1.0506782	-2.6036454
				H	-0.9858312	-2.8144734

				C	-3.7158592	2.0560046	-0.6681776
				C	-4.5372082	3.1659526	-0.4683836
				H	-4.1162942	4.1129056	-0.1456126
				C	-5.9032112	3.0481456	-0.7306376
				H	-6.5647512	3.8992916	-0.6044786
				C	-6.3944842	1.8257796	-1.1722996
				H	-7.4480262	1.7034396	-1.3999026
				C	-5.5199102	0.7413106	-1.3441806
				C	-6.0419372	-0.6367754	-1.7431596
				H	-6.8612642	-0.5014344	-2.4593136
				H	-5.2370142	-1.1777384	-2.2506256
				C	-5.6032472	-2.1950914	0.1859734
				H	-4.8320902	-2.6326104	-0.4552736
				H	-6.1532852	-3.0155074	0.6622084
				C	-4.9158722	-1.3771714	1.2764444
				C	-5.5430412	-1.1349404	2.5088364
				H	-6.4980872	-1.6024494	2.7235154
				C	-4.9308932	-0.3133354	3.4477864
				H	-5.3978892	-0.1265334	4.4095884
				C	-3.6954882	0.2574546	3.1362364
				H	-3.1811132	0.8880926	3.8543424
				C	-3.1192712	-0.0268614	1.8980144
				C	-1.7476512	0.4694146	1.5197414
				H	-1.1007152	0.5252886	2.3991554
				H	-1.3210342	-0.2218484	0.7926504
				C	-2.2201282	2.1397616	-0.5074646
				H	-1.7372302	1.4296506	-1.1768856
				H	-1.8681022	3.1483806	-0.7405036
				C	-7.7794922	-1.0299894	-0.0221646
				H	-7.6756972	-0.1587884	0.6484824
				H	-8.1994662	-1.8545414	0.5633944
				H	-8.5117062	-0.7709314	-0.7942516
				C	-1.9332722	2.9559096	1.8566024
				H	-3.0016432	2.9384466	2.0702744
				H	-1.6593682	3.9169106	1.4194884
				H	-1.3684842	2.7978286	2.7762894
				H	-0.5919852	1.8754936	0.6774514
TS5	frequency=-398.64 cm ⁻¹			7			
Pd	2.7436187	1.0738799	-0.3837841	Pd	-3.2060182	-1.2041625	-0.5473097
N	3.8796337	-0.7020421	-1.3550391	N	-4.9642872	0.2046415	-1.2328597
N	4.6255267	2.0297409	-0.8739731	N	-4.9148802	-2.2606145	0.2759253
N	2.6059917	-2.7919451	0.9431499	N	-3.1656162	2.9955965	-0.5405367
C	2.0306517	2.6821589	0.7036139	C	-1.8641252	-2.4552275	0.3746153
H	1.1582057	3.1045769	0.2078309	H	-0.8781032	-2.0322125	0.2007113
H	2.8187597	3.4262719	0.8000999	H	-1.9516432	-3.4606945	-0.0353837
H	1.7778917	2.2692899	1.6813919	H	-2.1253392	-2.4218025	1.4340353
C	3.6547287	-2.0302151	-1.2358541	C	-4.9344102	1.5277255	-1.4883827
C	4.5754997	-2.9579521	-1.7390241	C	-6.1141752	2.2843715	-1.5052347
H	4.3499457	-4.0166581	-1.6734631	H	-6.0574132	3.3453155	-1.7223877
C	5.7665117	-2.5201611	-2.3071021	C	-7.3309152	1.6747095	-1.2313177
H	6.4889447	-3.2293671	-2.6983641	H	-8.2542762	2.2448475	-1.2496447
C	6.0247457	-1.1509001	-2.3459661	C	-7.3428472	0.3171555	-0.9040527
H	6.9550847	-0.7679431	-2.7521091	H	-8.2685122	-0.1874715	-0.6477037
C	5.0543917	-0.2762141	-1.8637561	C	-6.1389142	-0.3789535	-0.9061737
C	5.2637737	1.2133769	-1.9652541	C	-6.0939552	-1.8490945	-0.5658257
H	6.3336887	1.4490219	-2.0005221	H	-7.0180132	-2.1542695	-0.0607097
H	4.8325877	1.5658919	-2.9071821	H	-6.0260102	-2.4299295	-1.4915177
C	2.4217967	-2.5079871	-0.4785021	C	-3.6014132	2.2144755	-1.7169437
H	1.6306457	-1.7707571	-0.5956211	H	-2.8487702	1.4792185	-2.0216497
H	2.0763297	-3.4353111	-0.9498661	H	-3.7378562	2.9214505	-2.5401187
C	4.5559517	3.4394409	-1.3742901	C	-4.8679452	-3.7543685	0.2777943
H	5.5695577	3.8022229	-1.5786331	H	-5.7728062	-4.1503465	0.7525763
H	4.0975997	4.0849519	-0.6277481	H	-3.9966942	-4.0980095	0.8330953
C	3.4414247	-3.9376851	1.2701309	C	-2.3353322	4.1361525	-0.9444967
H	3.2728257	-4.2209181	2.3141899	H	-2.1030752	4.7484945	-0.0691277
H	3.1458537	-4.7892331	0.6488569	H	-1.3831482	3.8430735	-1.4217937
N	4.0803757	0.2030769	1.2904609	N	-3.7410842	0.1836205	1.2565313
C	3.9093427	-0.9118911	2.0347119	C	-3.4843662	1.4992075	1.4107813
C	4.9419357	-1.3829071	2.8565189	C	-4.1688992	2.2585555	2.3694983
H	4.7691397	-2.2529141	3.4805909	H	-3.9335062	3.3121725	2.4709093

C	6.1759497	-0.7420701	2.8594199	C	-5.1472382	1.6662895	3.1556043
H	6.9849367	-1.0996881	3.4884689	H	-5.6808452	2.2405035	3.9062773
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H	2.5528547	1.5603239	-2.9101851	H	-3.6512292	-3.2679995	-2.1143507
H	0.9329237	1.2479069	-2.2069341	H	-3.4604762	-1.7410665	-3.0390597
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C	-3.5905827	1.2725217	0.0244348	C	1.8631745	-1.7361063	-1.2628046
H	-3.8318047	2.3416127	0.0652438	H	0.9832415	-2.3709743	-1.1853366
H	-4.0471857	0.7789877	0.8811638	H	2.5128915	-2.1689813	-2.0327166
C	3.8998913	-1.1212193	-0.0563342	C	-3.4836495	1.6304927	0.0000174
H	3.8661713	-0.0186333	-0.0034472	H	-3.6753385	2.7119827	0.0000394
H	4.4653993	-1.4779813	0.8115898	H	-3.9474665	1.1937517	0.8845664
N	0.1641433	-0.0625313	1.4020328	C	3.9351945	-1.2398973	-0.0000236
C	1.4006173	-0.5040663	1.7202108	H	3.9815815	-0.1377163	0.0000004
C	2.2634673	0.2986327	2.4805718	H	4.4758295	-1.5975953	0.8827944
H	3.2346603	-0.0914303	2.7652838	N	0.2138125	0.1142317	1.3977454
C	1.8761603	1.5808227	2.8517408	C	1.4422415	-0.3458953	1.7253464
H	2.5389253	2.2128567	3.4345808	C	2.3592115	0.4598317	2.4121804

C	0.6268973	2.0500667	2.4464748	H	3.3178635	0.0441447	2.7027574
H	0.2986993	3.0548167	2.6914358	C	2.0376485	1.7797177	2.7050674
C	-0.2030567	1.1924597	1.7285098	H	2.7374015	2.4188907	3.2343284
C	-1.6026827	1.6227067	1.3500148	C	0.8054345	2.2714907	2.2831874
H	-1.6754367	2.7175657	1.3412128	H	0.5266725	3.3053657	2.4581704
H	-2.2919827	1.2637947	2.1215998	C	-0.0813155	1.4095107	1.6375104
C	1.8709253	-1.8486183	1.1710458	C	-1.4504345	1.9217067	1.2452994
H	1.0115083	-2.5046013	1.0287148	H	-1.4273685	3.0190697	1.1837744
H	2.5384033	-2.3006833	1.9150098	H	-2.1468995	1.6727287	2.0534664
H	-4.0034137	0.8496507	-0.8905812	C	1.8631695	-1.7361623	1.2627214
H	4.4693263	-1.3933213	-0.9518862	H	0.9832335	-2.3710253	1.1852274
C	-2.7273947	-1.5276393	-1.5262582	H	2.5128855	-2.1690703	2.0326144
H	-3.7504667	-1.4846393	-1.1529302	H	-3.9474375	1.1937937	-0.8845686
H	-2.5614727	-0.8186413	-2.3400572	H	4.4758365	-1.5975563	-0.8828536
H	-2.4579467	-2.5336473	-1.8418562	H	-0.6699115	-3.2695003	0.8979834
O	-0.6768377	-2.8248043	-0.1685512	C	-2.7866265	-1.3806473	-1.4771596
H	-1.3963507	-3.4626343	-0.0611522	H	-3.6824065	-1.8576473	-1.0823046
				H	-3.0367105	-0.4322473	-1.9557966
				H	-2.2857165	-2.0367293	-2.1890616
9				9_Iso			
Pd	0.2659467	-1.4497311	-1.5086585	Pd	1.9447242	-1.1412167	-0.0506947
N	0.0665297	-1.3060581	0.6029665	N	0.1331372	-0.5249007	1.1686703
N	0.0261317	0.7885119	-1.3459575	N	2.2691562	1.0428053	0.1683873
N	2.9263087	0.3507719	0.1965715	N	-2.3124818	-2.0365607	-0.6467267
N	-2.9527563	-0.1838311	-0.2411855	C	3.6489882	-1.5458957	-1.0900147
C	0.4680677	-3.4772471	-1.5441085	H	3.7660992	-0.8266067	-1.9120147
H	-0.5255433	-3.9293511	-1.6433905	H	3.6216702	-2.5499467	-1.5280687
H	0.9436797	-3.8472001	-0.6274045	H	4.5205592	-1.4833967	-0.4266967
H	1.0665407	-3.7257601	-2.4220705	C	-1.0422798	-1.1636317	1.3573463
C	-1.1571843	-1.2981331	1.1813575	C	-1.9574398	-0.6939847	2.3109023
C	-1.2970813	-1.1442551	2.5637885	H	-2.8671148	-1.2551607	2.4951253
H	-2.2885293	-1.1706251	3.0041115	C	-1.6994748	0.4866093	2.9999643
C	-0.1663923	-0.9708051	3.3561475	H	-2.4029358	0.8631303	3.7370523
H	-0.2553913	-0.8627631	4.4332505	C	-0.5345098	1.1923323	2.7083483
C	1.0804567	-0.9343231	2.7391635	H	-0.3149888	2.1404693	3.1894503
H	1.9860327	-0.7926811	3.3200275	C	0.3621982	0.6452823	1.7906413
C	1.1732927	-1.0908391	1.3531235	C	1.6815952	1.3352803	1.5057673
C	2.5224987	-0.9810481	0.6457455	H	1.5735262	2.4218503	1.6524963
H	3.2940047	-1.3314551	1.3449355	H	2.4096912	0.9817273	2.2437443
H	2.5138457	-1.6456911	-0.2228795	C	-1.3843628	-2.3440907	0.4511763
C	2.4785387	0.8555579	-1.1022565	H	-0.4569278	-2.7608187	0.0415993
H	2.4566767	0.0215469	-1.8098705	H	-1.8651118	-3.1184997	1.0634123
H	3.2339357	1.5769449	-1.4428735	C	3.7128572	1.3786123	0.2162583
C	1.1200377	1.5518199	-1.1389985	H	3.8646652	2.4457813	0.4417213
C	1.0065767	2.9318019	-0.9391845	H	4.1687642	1.1471423	-0.7459527
H	1.9020907	3.5295499	-0.8022985	C	-3.6640908	-1.6741567	-0.2746287
C	-0.2548273	3.5211289	-0.9310875	H	-3.7831198	-0.6691887	0.1696063
H	-0.3634173	4.5925949	-0.7886765	H	-4.3089948	-1.7203967	-1.1608267
C	-1.3746963	2.7133089	-1.1095485	N	-0.1693988	0.4016313	-1.5303917
H	-2.3742673	3.1361539	-1.1080205	C	-1.4615468	0.1022583	-1.7026507
C	-1.2054033	1.3388059	-1.3063005	C	-2.4527298	1.0982623	-1.6651997
C	-2.4072833	0.4098769	-1.4613915	H	-3.4902218	0.8481063	-1.8634497
H	-3.2180693	0.9857089	-1.9285395	C	-2.0803988	2.4068933	-1.3708607
H	-2.1280563	-0.4030091	-2.1385325	H	-2.8244588	3.1978823	-1.3380137
C	-2.3836493	-1.4252301	0.2825765	C	-0.7396818	2.6872473	-1.0971067
H	-2.1227513	-2.0649321	-0.5653965	H	-0.4223128	3.6902383	-0.8270467
H	-3.1738353	-1.9207561	0.8628455	C	0.1866572	1.6450913	-1.1903847
C	3.1117737	1.3448529	1.2338035	C	1.6629602	1.8654943	-0.9297047
H	2.1812507	1.7439239	1.6745925	H	1.8437062	2.9309343	-0.7159307
H	3.6752147	2.1928899	0.8269505	H	2.2179502	1.6047303	-1.8353167
H	3.7064887	0.9148689	2.0485185	C	-1.7824788	-1.3837177	-1.8455557
C	-3.4664413	0.7472349	0.7428415	H	-0.8567568	-1.8922207	-2.1261277
H	-2.6983263	1.2990579	1.3126655	H	-2.5205898	-1.5292017	-2.6460167
H	-4.0907363	0.2068219	1.4642185	H	4.1988472	0.7716403	0.9803013
H	-4.1039423	1.4869849	0.2442675	H	-4.0466848	-2.4011077	0.4522493
O	0.5644027	-1.5648531	-3.4815745	O	1.5051272	-3.0764197	-0.0374517
H	0.2382577	-0.7201391	-3.8242655	H	2.1482122	-3.5403147	-0.5873897
TS10_N ₃ +N ₃	frequency=-272.91 cm ⁻¹			TS10_N ₃ +N ₂	frequency=-262.44 cm ⁻¹		
Pd	2.1869677	0.2516987	-0.9678852	Pd	-2.2134663	-0.6369675	0.7890320
N	3.2005297	-0.6538403	0.9188888	N	-3.2226753	0.0531165	-1.1776040

N	3.0764327	-1.6008843	-1.7898232	N	-3.2535243	-2.4772555	0.1693550
N	4.5125297	2.2828197	1.9240088	N	-4.3274483	2.9772305	0.0988420
C	1.5160317	0.9674387	-2.7578792	C	-1.5518053	-1.4094565	2.5587210
H	0.7578137	1.7394037	-2.6029322	H	-0.9494893	-0.6781615	3.1037500
H	1.0821497	0.1680117	-3.3642372	H	-0.9550003	-2.3122615	2.4002430
H	2.3814657	1.4027497	-3.2678602	H	-2.4403683	-1.6482515	3.1530730
C	3.5750487	-0.0566483	2.0727988	C	-3.5257043	1.2989795	-1.6086490
C	4.2360647	-0.7881313	3.0703108	C	-4.2015413	1.4860305	-2.8232800
H	4.4811227	-0.3014043	4.0080268	H	-4.3869033	2.4951745	-3.1747010
C	4.5819867	-2.1156413	2.8474588	C	-4.6369683	0.3879615	-3.5556670
H	5.0995637	-2.6900263	3.6097648	H	-5.1659473	0.5209565	-4.4944500
C	4.2736867	-2.6892783	1.6158858	C	-4.4045143	-0.8886405	-3.0481450
H	4.5594147	-3.7103473	1.3848098	H	-4.7629193	-1.7725055	-3.5657020
C	3.5759997	-1.9258753	0.6811018	C	-3.6879373	-1.0128225	-1.8591140
C	3.1566137	-2.5437173	-0.6341672	C	-3.3533743	-2.3858725	-1.3185750
H	3.8218517	-3.3827813	-0.8820292	H	-4.0785193	-3.1224805	-1.6916960
H	2.1526827	-2.9647543	-0.5100522	H	-2.3740513	-2.6809025	-1.7111450
C	3.3523597	1.4439907	2.2378298	C	-3.2079033	2.4936055	-0.7131790
H	2.5219997	1.7646547	1.6068398	H	-2.3861973	2.2411185	-0.0409210
C	3.0932967	1.6348307	3.2871248	H	-2.8949683	3.3259745	-1.3565010
C	2.2669547	-2.2666983	-2.8448242	C	-2.5164343	-3.7286255	0.4926630
H	2.7193507	-3.2249663	-3.1345532	H	-3.0409293	-4.6052325	0.0887370
H	2.2117537	-1.6264203	-3.7243912	H	-2.4323833	-3.8348085	1.5735550
C	5.6550517	2.1757817	2.8097428	C	-5.4344353	3.5907245	-0.6074070
H	6.2525297	1.2527457	2.7035838	H	-6.0931383	2.8934185	-1.1550590
H	6.3265027	3.0249467	2.6377478	H	-6.0578593	4.1406685	0.1069650
N	4.7951427	0.6656407	-1.0077752	N	-4.8137743	-0.1733075	1.1558920
C	5.5398147	1.4780867	-0.2428432	C	-5.4837873	0.9882505	1.1511190
C	6.9204657	1.2643137	-0.1003832	C	-6.8671263	1.0195295	0.9111180
H	7.5208857	1.9602637	0.4761468	H	-7.4071203	1.9591995	0.9638970
C	7.5026967	0.1522667	-0.7014102	C	-7.5304503	-0.1642205	0.6020680
H	8.5676697	-0.0346193	-0.6007332	H	-8.5989933	-0.1630825	0.4086980
C	6.6968167	-0.7316933	-1.4217772	C	-6.8017913	-1.3531945	0.5269260
H	7.1137997	-1.6247993	-1.8768432	H	-7.2836343	-2.2884575	0.2592240
C	5.3415067	-0.4275283	-1.5555782	C	-5.4384323	-1.3095215	0.8214040
C	4.4192187	-1.2951053	-2.3887282	C	-4.5948013	-2.5681795	0.8396140
H	4.9210777	-2.2395603	-2.6424362	H	-5.1569293	-3.4037085	0.3995940
H	4.2126847	-0.7734623	-3.3287582	H	-4.3882693	-2.8278285	1.8826620
C	4.8015287	2.5769807	0.5180898	C	-4.6572533	2.2592975	1.3320050
H	3.8484757	2.7653537	0.0179228	H	-3.7177833	1.9925745	1.8222710
H	5.4028677	3.4952327	0.4943178	H	-5.2073593	2.9565555	1.9773360
H	1.2575897	-2.4468783	-2.4727812	H	-1.5147693	-3.6824955	0.0638360
H	5.3135817	2.2315747	3.8499148	H	-5.0455963	4.3162725	-1.3313690
C	0.0143637	-0.5557913	-0.4851682	C	0.0182187	-0.9878815	-0.2404960
H	-0.1042583	0.3732467	0.0423798	H	0.0477217	0.0511035	0.0435690
H	-0.3104163	-0.6643173	-1.5065502	H	0.2727937	-1.7646455	0.4626260
H	0.3573017	-1.4258533	0.0491058	H	-0.4258503	-1.2664205	-1.1828140
Pd	-2.4608263	-1.1167073	0.2412728	Pd	2.3293367	-0.7919185	-1.0061840
N	-3.6519373	0.6536257	1.3517498	N	3.4892177	1.2558055	-0.7867390
N	-4.0844103	-0.2334483	-1.2399032	N	3.8013927	-1.0640075	0.8261270
N	-2.3406963	2.6593817	-1.0178782	N	2.0956917	1.4977875	2.2425850
N	-4.7508153	-2.0701013	0.9704408	N	5.9777227	-0.8363565	-1.6956900
C	-1.3890313	-1.8138423	1.8407358	C	1.3928577	-0.3325525	-2.7694080
H	-0.7833563	-0.9948633	2.2410328	H	0.8184657	0.5852805	-2.6109840
H	-0.7473233	-2.6698283	1.6175668	H	0.7387807	-1.1222125	-3.1447100
H	-2.1291893	-2.1131793	2.5915978	H	2.1784407	-0.1437555	-3.5081600
C	-1.9081973	-2.7673903	-0.8417652	C	1.9464867	-2.7742795	-1.4017030
H	-0.9318343	-3.1856463	-0.5861632	H	0.9238147	-2.9956475	-1.7123320
H	-1.9248413	-2.4910743	-1.9017632	H	2.1890707	-3.3377835	-0.4948810
H	-2.6698893	-3.5315293	-0.6572642	H	2.6201717	-3.0654325	-2.2143620
C	-4.8286863	0.2883317	1.9036988	C	4.6483187	1.3318935	-1.4827110
C	-5.7466163	1.2267417	2.3821748	C	5.4676357	2.4632975	-1.4132890
H	-6.6808733	0.8904827	2.8198228	H	6.3711447	2.5049525	-2.0122390
C	-5.4435173	2.5821167	2.2981798	C	5.1100157	3.5234035	-0.5874050
H	-6.1301283	3.3291297	2.6847328	H	5.7258437	4.4159155	-0.5300620
C	-4.2511323	2.9556717	1.6899118	C	3.9459567	3.4114815	0.1644270
H	-3.9819653	4.0013307	1.5864078	H	3.6322187	4.2108575	0.8274850
C	-3.3877873	1.9698647	1.1960918	C	3.1576257	2.2604575	0.0553590
C	-2.1494813	2.3730507	0.4082198	C	1.9174407	2.1152215	0.9265150
H	-1.7317663	3.2817787	0.8568868	H	1.5123507	3.1183405	1.1050970

H	-1.3991273	1.5916987	0.5082058	H	1.1473107	1.5642905	0.3885340
C	-2.5252813	1.5437527	-1.9503742	C	2.1789907	0.0412175	2.3509370
H	-1.7852083	0.7801077	-1.7166142	H	1.4302617	-0.3893475	1.6901740
H	-2.3085903	1.9312317	-2.9537982	H	1.8939837	-0.2156575	3.3794900
C	-3.8992513	0.8850077	-1.9754542	C	3.5269777	-0.6173195	2.0736630
C	-4.9480103	1.4702317	-2.6946822	C	4.4617217	-0.7221625	3.1094260
H	-4.7533003	2.3392157	-3.3139472	H	4.1929177	-0.3845235	4.1047020
C	-6.2278763	0.9360447	-2.5964052	C	5.7148477	-1.2684425	2.8560340
H	-7.0578773	1.3757447	-3.1410532	H	6.4476027	-1.3727365	3.6505660
C	-6.4267833	-0.1610283	-1.7639132	C	6.0072047	-1.6738305	1.5586100
H	-7.4162383	-0.5854683	-1.6282692	H	6.9760677	-2.0947425	1.3112910
C	-5.3335673	-0.7258453	-1.1018952	C	5.0379617	-1.5467955	0.5581400
C	-5.5570473	-1.9650413	-0.2503782	C	5.3989217	-1.9023055	-0.8811820
H	-6.6362753	-2.0467243	-0.0330422	H	6.1317077	-2.7183955	-0.8532470
H	-5.3024883	-2.8342183	-0.8685402	H	4.5112237	-2.2766665	-1.3939850
C	-5.1450323	-1.1874473	2.0730628	C	5.0938077	0.1391915	-2.3288540
C	-3.0975803	3.8633187	-1.3195222	H	4.2125617	-0.3959585	-2.6917930
H	-4.1805393	3.7983717	-1.1190612	H	5.6235677	0.5325195	-3.2060930
H	-2.9689673	4.1147207	-2.3782182	C	2.9034617	2.2503765	3.1875080
H	-2.6987653	4.6966107	-0.7307582	H	3.9866277	2.2502525	2.9798760
O	1.4932417	1.9250007	-0.1118592	H	2.7565807	1.8435345	4.1943190
H	1.1116057	2.4929357	-0.7946092	H	2.5657137	3.2923505	3.2005830
H	-6.2190223	-1.2890423	2.3074488	C	7.2840077	-0.3522065	-1.2876380
H	-4.6031433	-1.5370633	2.9600748	H	7.2851177	0.2918225	-0.3920160
C	-4.7094563	-3.4621183	1.4364918	H	7.7310767	0.2181645	-2.1094850
H	-4.0099813	-3.5475063	2.2710478	H	7.9391537	-1.2068365	-1.0863110
H	-5.6960743	-3.8272903	1.7669758	O	-1.3412373	1.1118995	1.2402610
H	-4.3556333	-4.1101063	0.6318978	H	-0.9367483	1.0710085	2.1174350
8_N ₂				TS8_N ₂ N ₂ frequency=-311.18 cm ⁻¹			
Pd	1.8734402	-0.4382249	0.0305879	Pd	-1.2403196	-1.2325517	-0.0411721
N	0.0521932	0.0163071	-1.4343021	N	0.1710684	0.0742743	1.3732139
N	0.0213512	-0.0574579	1.4250799	N	0.2104814	0.1024943	-1.3799581
N	-1.3290688	-2.7266329	-0.0439481	N	2.7572094	-1.6696557	-0.0123971
N	0.3852352	2.9932161	0.0492639	N	-2.2356866	1.8858473	-0.0022701
C	3.4202382	0.1196441	-1.2104841	C	-2.8162626	-1.6034767	1.2173439
H	3.6666022	1.1222681	-0.8519331	H	-3.4944846	-0.7822337	0.9715249
H	3.0033792	0.1380341	-2.2185261	H	-2.4290816	-1.5201927	2.2337809
H	4.3024972	-0.5136719	-1.1647591	H	-3.3087966	-2.5605267	1.0622329
C	3.1828382	-0.5678499	1.6006839	C	-2.3658476	-1.9621897	-1.5813471
H	4.2219102	-0.5984209	1.2759979	H	-3.0464946	-2.7588957	-1.2876651
H	2.9289352	-1.4609179	2.1744329	H	-1.6643806	-2.3065147	-2.3437241
H	2.9909602	0.3287151	2.1948399	H	-2.9302576	-1.0965867	-1.9379021
C	-0.1855588	1.3074701	-1.7723571	C	-0.2654306	1.3401493	1.5813139
C	-1.2851618	1.6688001	-2.5560651	C	0.5719964	2.3322463	2.0942709
H	-1.4234278	2.7086891	-2.8321701	H	0.1828984	3.3327993	2.2471029
C	-2.1791978	0.6921991	-2.9804821	C	1.8852794	2.0146543	2.4302919
H	-3.0291408	0.9488061	-3.6052531	H	2.5434904	2.7613833	2.8634069
C	-1.9590368	-0.6208279	-2.5807641	C	2.3303964	0.7193333	2.2013389
H	-2.6364788	-1.4133579	-2.8800651	H	3.3437344	0.4273623	2.4538789
C	-0.8457958	-0.9332409	-1.7937781	C	1.4647234	-0.2249227	1.6344599
C	-0.6742918	-2.3671209	-1.2979881	C	2.0073954	-1.5946627	1.2427459
H	-1.0801208	-3.0323299	-2.0697791	H	2.6833354	-1.9365927	2.0346849
H	0.3853712	-2.5971169	-1.2096991	H	1.1850174	-2.3053577	1.1972389
C	-0.6882678	-2.4214709	1.2297359	C	2.0252794	-1.5706327	-1.2747381
H	0.3800602	-2.6297509	1.1411439	H	1.1845764	-2.2673427	-1.2511721
H	-1.0901458	-3.1234629	1.9704799	H	2.7035234	-1.9120137	-2.0650581
C	-0.8724398	-1.0097259	1.7738159	C	1.5020444	-0.1892447	-1.6446491
C	-1.9739548	-0.7071459	2.5797819	C	2.3666974	0.7698373	-2.1871501
H	-2.6567248	-1.4986909	2.8695939	H	3.3824494	0.4894873	-2.4432701
C	-2.1719458	0.6000681	3.0123189	C	1.9133454	2.0676093	-2.3887551
H	-3.0116108	0.8509401	3.6530999	H	2.5694284	2.8270383	-2.8026041
C	-1.2712198	1.5797781	2.6058219	C	0.5954284	2.3727703	-2.0559131
H	-1.3937358	2.6119771	2.9159189	H	0.2015274	3.3735463	-2.1947831
C	-0.1871498	1.2265571	1.7978479	C	-0.2384356	1.3661383	-1.5669821
C	0.7581852	2.3094131	1.2801969	C	-1.7089496	1.6504303	-1.3498791
H	0.8546792	3.0721771	2.0633679	H	-1.9437216	2.5460823	-1.9420541
H	1.7588482	1.8829731	1.1363059	H	-2.2588886	0.8335453	-1.8458391
C	0.7336412	2.4016171	-1.2372131	C	-1.7272186	1.6546523	1.3544969
H	1.7546562	2.0226131	-1.1684911	H	-2.2983056	0.8558083	1.8511079
H	0.7488302	3.2154011	-1.9718851	H	-1.9434816	2.5631153	1.9333929

C	-2.7821858	-2.7223579	-0.0475721	C	4.0805794	-1.0648277	-0.0001641
H	-3.2451408	-1.7218719	-0.0245051	H	4.0895974	0.0378683	0.0095179
H	-3.1470588	-3.2807959	0.8211659	H	4.6358624	-1.3972867	-0.8834301
H	-3.1426228	-3.2382989	-0.9438151	H	4.6264394	-1.4129287	0.8828449
C	-0.8258668	3.7951671	0.0920749	C	-0.9225266	-3.2415397	0.3772289
H	-1.7649468	3.2178891	0.0828199	H	-0.6914746	-3.2986637	1.4400329
H	-0.8391288	4.4734101	-0.7674241	H	-1.7827116	-3.8568887	0.1313999
H	-0.8188778	4.4119541	0.9971409	H	-0.0702296	-3.5040657	-0.2481171
C	2.6941282	-2.2835239	-0.4721011	C	-3.6646666	2.1524853	-0.0184671
H	2.5481262	-2.4072839	-1.5443411	H	-3.9235346	2.7769433	-0.8806331
H	3.7441462	-2.3583539	-0.2052391	H	-4.2862836	1.2407553	-0.0714061
H	2.1000522	-2.9861809	0.1114249	H	-3.9563326	2.7011353	0.8826479
Me Radical Path				Int12(T)			
TS11(S) frequency=-112.93 cm ⁻¹							
N	-3.5920723	0.3439572	-1.3329834	N	3.5232085	-0.7565875	-1.1946117
N	-4.2143663	-2.3754398	-0.4783754	N	4.1652965	2.0838875	-1.2160607
N	-2.4324353	2.8323832	0.6009536	N	2.4378205	-2.4810695	1.4936793
C	-3.4608583	1.6857952	-1.4095124	C	3.4247175	-2.0458105	-0.8109817
C	-4.4506663	2.4790132	-2.0033194	C	4.4174945	-2.9770025	-1.1420427
H	-4.2938383	3.5482812	-2.0971944	H	4.2906505	-4.0174595	-0.8628117
C	-5.6264353	1.8883332	-2.4532074	C	5.5566045	-2.5538305	-1.8184107
H	-6.4091773	2.4857342	-2.9108284	H	6.3394885	-3.2586585	-2.0815167
C	-5.7902263	0.5166852	-2.2820234	C	5.6856095	-1.2025495	-2.1331077
H	-6.7075443	0.0213942	-2.5839034	H	6.5745035	-0.8264625	-2.6292047
C	-4.7484313	-0.2265898	-1.7226484	C	4.6450315	-0.3315795	-1.8072167
C	-4.8965903	-1.7336068	-1.6135654	C	4.7313215	1.1319605	-2.1945627
H	-5.9693943	-1.9879168	-1.6280654	H	5.7777085	1.3855295	-2.4271477
H	-4.4672483	-2.1702188	-2.5224864	H	4.1611315	1.2657785	-3.1204877
C	-2.2401093	2.3224902	-0.7611114	C	2.2259215	-2.4353515	0.0424383
H	-1.4245713	1.5968882	-0.7285884	H	1.4144555	-1.7337515	-0.1640447
H	-1.9236263	3.1720922	-1.3787184	H	1.8954025	-3.4368405	-0.2587337
C	-3.9936703	-3.8005938	-0.7784964	C	3.9064905	3.3782045	-1.8765677
H	-4.9409613	-4.3461998	-0.9144174	H	4.8392945	3.8541195	-2.2158307
H	-3.4398293	-4.2670508	0.0378956	H	3.4007565	4.0472875	-1.1788497
C	-3.3491553	3.9461362	0.7573956	C	3.3258895	-3.5255735	1.9728373
H	-4.4188253	3.6921662	0.6602006	H	4.3981445	-3.3570855	1.7726523
H	-3.2027473	4.3995122	1.7444006	H	3.2033755	-3.6371505	3.0560343
C	-3.6117923	1.0481222	1.9630816	C	3.7369345	-0.4120675	2.1759103
C	-4.6866903	1.5756932	2.6901666	C	4.8418035	-0.7119265	2.9822523
H	-4.5872573	2.5474102	3.1619416	H	4.7559635	-1.4759235	3.7475983
C	-5.8689363	0.8516222	2.7888536	C	6.0388855	-0.0324525	2.7834383
H	-6.7162383	1.2430032	3.3436546	H	6.9102355	-0.2531215	3.3924673
C	-5.9518743	-0.3789758	2.1420466	C	6.1046835	0.9246205	1.7738443
H	-6.8674023	-0.9609368	2.1654856	H	7.0282435	1.4556425	1.5669763
C	-4.8334803	-0.8674898	1.4638896	C	4.9564875	1.2043435	1.0304083
C	-4.8959273	-2.2401038	0.8209946	C	4.9920105	2.3047715	-0.0129767
H	-5.9508743	-2.5525378	0.7498216	H	6.0387685	2.5072615	-0.2897717
H	-4.4063903	-2.9454848	1.5023866	H	4.6119255	3.2174295	0.4596553
C	-2.3657233	1.8862802	1.7145636	C	2.4576625	-1.2316695	2.2592903
H	-1.5232473	1.2213572	1.5264576	H	1.6295405	-0.6010015	1.9284203
H	-2.1497523	2.4667362	2.6203736	H	2.2816815	-1.4989525	3.3086623
H	-3.4000963	-3.8938728	-1.6898544	H	3.2565925	3.2243735	-2.7384447
H	-3.1193433	4.7100322	0.0061986	H	3.0458335	-4.4778685	1.5090213
Pd	2.1046167	1.0866142	-0.1512234	Pd	-2.2004475	-1.0689085	-0.4607347
N	3.5919587	-0.3439298	-1.3332744	N	-3.5299985	0.7744655	-1.1680417
N	4.2143367	2.3754492	-0.4786744	N	-4.3592285	-2.0275475	-1.1758967
N	2.4324697	-2.8323858	0.6007106	N	-2.2773355	2.4551185	1.4580223
C	1.1962337	2.4540792	1.0826906	C	-1.4586455	-2.8416445	0.2908203
H	1.1080337	1.9796412	2.0664696	H	-1.0792495	-2.6386585	1.2973343
H	0.2167017	2.7752102	0.7323476	H	-0.6677045	-3.2725035	-0.3233737
H	1.8625997	3.3189002	1.1607176	H	-2.2884015	-3.5515235	0.3648693
C	3.4607277	-1.6857658	-1.4098194	C	-3.3264245	2.0608395	-0.8108527
C	4.4504807	-2.4789798	-2.0037254	C	-4.2634775	3.0552195	-1.1225677
H	4.2936347	-3.5482438	-2.0976104	H	-4.0493805	4.0876985	-0.8679577
C	5.6262177	-1.8883008	-2.4536964	C	-5.4586525	2.7067415	-1.7406437
H	6.4089177	-2.4856988	-2.9113934	H	-6.1998775	3.4619445	-1.9841907
C	5.7900347	-0.5166578	-2.2824964	C	-5.6971325	1.3633885	-2.0196167
H	6.7073327	-0.0213688	-2.5844394	H	-6.6321675	1.0423575	-2.4672677
C	4.7482907	0.2266152	-1.7230214	C	-4.7067205	0.4251475	-1.7244517
C	4.8964737	1.7336282	-1.6139224	C	-4.9264855	-1.0272985	-2.0990127

H	5.9692797	1.9879272	-1.6284934	H	-6.0043945	-1.1995005	-2.2513677
H	4.4670737	2.1702612	-2.5228064	H	-4.4440095	-1.1940535	-3.0688237
C	2.2400297	-2.3224638	-0.7613274	C	-2.0863885	2.3924115	0.0064753
H	1.4245007	-1.5968568	-0.7287184	H	-1.3125045	1.6495405	-0.1868787
H	1.9234867	-3.1720508	-1.3789244	H	-1.7158245	3.3745215	-0.3132877
C	3.9936247	3.8006082	-0.7787554	C	-4.2454125	-3.3220665	-1.8726227
H	4.9409077	4.3462152	-0.9147274	H	-5.2315385	-3.7210025	-2.1575847
H	3.4398357	4.2670522	0.0376796	H	-3.7489885	-4.0464645	-1.2252827
C	3.3491907	-3.9461538	0.7570486	C	-3.1410935	3.5075435	1.9559513
H	4.4188547	-3.6921958	0.6597596	H	-4.2213885	3.3519225	1.7879723
H	3.2028667	-4.3995448	1.7440596	H	-2.9869165	3.6221385	3.0350963
N	3.6734527	0.1808202	1.4088886	N	-3.7230075	-0.5532475	1.2841713
C	3.6119637	-1.0481598	1.9627666	C	-3.5609715	0.4142225	2.2133483
C	4.6869307	-1.5757558	2.6897306	C	-4.5945995	0.7432675	3.1007463
H	4.5875427	-2.5474868	3.1614846	H	-4.4203115	1.4913505	3.8667923
C	5.8691887	-0.8516898	2.7883236	C	-5.8317655	0.1214415	2.9795903
H	6.7165437	-1.2430898	3.3430306	H	-6.6469745	0.3693845	3.6526843
C	5.9520657	0.3789272	2.1415466	C	-6.0124265	-0.8107465	1.9608873
H	6.8675977	0.9608852	2.1649136	H	-6.9722625	-1.2940145	1.8095073
C	4.8336077	0.8674632	1.4635106	C	-4.9326575	-1.1294795	1.1353673
C	4.8959947	2.2400922	0.8206436	C	-5.1033245	-2.2118075	0.0843223
H	5.9509327	2.5525362	0.7493986	H	-6.1786375	-2.3524145	-0.1121707
H	4.4064997	2.9454542	1.5020856	H	-4.7428195	-3.1502045	0.5208543
C	2.3658667	-1.8863058	1.7143456	C	-2.2578045	1.2022935	2.2182803
H	1.5233797	-1.2213718	1.5263316	H	-1.4474415	0.5941325	1.8051653
H	2.1499747	-2.4667788	2.6201636	H	-2.0158275	1.4595765	3.2578003
H	3.3999937	3.8939052	-1.6900754	H	-3.6428195	-3.1995635	-2.7734497
H	3.1192997	-4.7100328	0.0058596	H	-2.8653945	4.4563555	1.4811283
C	1.1966117	1.9519372	-1.7702424	C	-1.2193265	-1.5525195	-2.2004027
H	0.4116967	1.2766232	-2.1085404	H	-0.1487835	-1.4426635	-2.0349467
H	0.7841947	2.9353082	-1.5387404	H	-1.4552825	-2.5702275	-2.5201317
H	1.9773427	2.0382072	-2.5337294	H	-1.5608515	-0.8275335	-2.9471187
Pd	-2.1046273	-1.0865998	-0.1510754	Pd	2.1382275	1.0053485	-0.4107987
C	-1.1961513	-2.4540788	1.0827556	C	1.3490685	2.7079565	0.4259993
H	-1.1078523	-1.9796418	2.0665256	H	2.1535985	3.1474565	1.0261263
H	-0.2166563	-2.7752288	0.7323246	H	0.5277665	2.3837865	1.0644453
H	-1.8625263	-3.3188868	1.1608466	H	0.9980185	3.4297895	-0.3135947
C	-1.1967513	-1.9518978	-1.7701794	C	1.0518895	1.4144365	-2.1068437
H	-0.7842973	-2.9352638	-1.5387194	H	0.0332455	1.0795535	-1.9241397
H	-0.4118763	-1.2765708	-2.1085434	H	1.5097165	0.8132875	-2.8998897
H	-1.9775473	-2.0381748	-2.5335974	H	1.0759395	2.4735215	-2.3699037
O	-0.0000053	0.0000072	0.0016226	O	-0.1051235	-0.0817745	0.3242193
H	0.0000407	-0.0000128	0.9712776	H	0.0435255	-0.8331685	0.9120243
N	-3.6733323	-0.1808428	1.4091746	N	3.7896385	0.5689115	1.2516423
13_N ₃ (D)				14(D)			
Pd	1.2577893	-0.0000364	-1.1414247	Pd	1.4987653	-1.0743549	-0.0194240
N	-0.0855457	-1.3998154	0.0044983	N	-0.1594257	0.0106581	1.3910430
N	2.2333983	0.0000616	0.9677663	N	2.0338313	1.4091901	0.0108660
N	-2.5364557	-0.0000774	-1.7906707	N	-2.4628767	-1.9377359	-0.0322530
C	2.3924143	1.4038016	-2.1231057	C	2.9114823	-1.6357919	-1.4005660
H	3.4583723	1.1770506	-2.0794727	H	3.8368253	-1.0609109	-1.2971780
H	2.1860683	2.3742206	-1.6633777	H	2.4531003	-1.4438749	-2.3767900
H	2.0650193	1.4094666	-3.1674117	H	3.1348983	-2.7009139	-1.3077180
C	-1.3317167	-1.7387494	-0.3825677	C	-1.3593107	-0.5135119	1.7247350
C	-2.1753357	-2.4482414	0.4794393	C	-2.3022347	0.2429781	2.4374540
H	-3.1604047	-2.7497644	0.1401083	H	-3.2361057	-0.2209319	2.7374930
C	-1.7404997	-2.7533514	1.7664993	C	-2.0397157	1.5748341	2.7338040
H	-2.3826767	-3.2995414	2.4503103	H	-2.7633907	2.1779601	3.2749050
C	-0.4740947	-2.3337124	2.1727313	C	-0.8381527	2.1284251	2.2998230
H	-0.1145157	-2.5332644	3.1768473	H	-0.6063997	3.1742881	2.4760600
C	0.3321573	-1.6583194	1.2574113	C	0.0827853	1.3116531	1.6395810
C	1.7488203	-1.2508874	1.6130143	C	1.4349663	1.8941871	1.2596800
H	1.8548253	-1.1790584	2.7045203	H	1.3569033	2.9961481	1.2661890
H	2.4197103	-2.0506654	1.2818523	H	2.1361633	1.6296811	2.0599980
C	-1.8048297	-1.2632534	-1.7540267	C	-1.7128357	-1.9118189	1.2290880
H	-0.9357227	-1.1794384	-2.4166047	H	-0.8046447	-2.5087779	1.0858010
H	-2.4638457	-2.0312984	-2.1763837	H	-2.3451487	-2.3918469	1.9888760
C	3.7153243	0.0000766	0.9248753	C	3.4808973	1.6557751	0.0187060
H	4.1396673	0.0000106	1.9383003	H	3.7269053	2.7315131	0.0504650
H	4.0634903	0.8862406	0.3935873	H	3.9288833	1.2221401	-0.8773950

C	-3.8516167	-0.0000414	-1.1724147	C	-3.7907817	-1.3655719	-0.0119440
H	-3.8461767	0.0000146	-0.0693667	H	-3.8385897	-0.2608969	0.0147860
H	-4.4073197	0.8828746	-1.5054957	H	-4.3415197	-1.6949239	-0.9019020
N	-0.0855587	1.3997906	0.0044283	N	-0.1698817	0.0660871	-1.4060550
C	-1.3317217	1.7387056	-0.3827057	C	-1.3771057	-0.4391669	-1.7409750
C	-2.1753537	2.4482716	0.4792213	C	-2.3276117	0.3487121	-2.4084420
H	-3.1604077	2.7497836	0.1398403	H	-3.2689597	-0.0983939	-2.7107410
C	-1.7405537	2.7534766	1.7662743	C	-2.0617517	1.6892941	-2.6587460
H	-2.3827477	3.2997326	2.4500193	H	-2.7903917	2.3161531	-3.1651190
C	-0.4741677	2.3338556	2.1725783	C	-0.8497537	2.2199291	-2.2243220
H	-0.1146177	2.5334886	3.1766873	H	-0.6145897	3.2702941	-2.3658650
C	0.3321013	1.6583806	1.2573323	C	0.0760813	1.3740801	-1.6090600
C	1.7487603	1.2509856	1.6130053	C	1.4370973	1.9321691	-1.2238330
H	1.8547043	1.1791526	2.7045163	H	1.3716883	3.0348731	-1.2032250
H	2.4196463	2.0507846	1.2818903	H	2.1317593	1.6777331	-2.0330770
C	-1.8048057	1.2630866	-1.7541327	C	-1.7260807	-1.8565609	-1.2989900
H	-0.9356827	1.1791916	-2.4166797	H	-0.8145937	-2.4563569	-1.1884690
H	-2.4637927	2.0311036	-2.1765877	H	-2.3650137	-2.3063389	-2.0716930
H	4.0634973	-0.8860054	0.3934553	H	3.9265713	1.1674951	0.8876150
H	-4.4073227	-0.8829894	-1.5054047	H	-4.3326187	-1.7369049	0.8669610
C	2.3923813	-1.4039324	-2.1230597	C	2.9026303	-1.6469969	1.3694570
H	3.4583423	-1.1771794	-2.0794907	H	3.9108683	-1.2971319	1.1304820
H	2.1860583	-2.3743284	-1.6632727	H	2.5678723	-1.2156719	2.3198770
H	2.0649423	-1.4096574	-3.1673527	H	2.8906273	-2.7362849	1.4416810
				O	0.6475603	-3.0833469	-0.0647100
				H	1.4203223	-3.6612329	-0.1169340
TS15(T) frequency=-418.93 cm ⁻¹				TS13_N3Na(D) frequency=-338.14 cm ⁻¹			
N	4.4067166	-0.7151824	-1.0746705	Pd	-0.9498735	-1.1344681	-0.0151684
N	3.8342356	2.1473336	-1.2102525	N	0.1846185	0.2903199	-1.3588074
N	3.0695506	-2.8801224	1.1155525	N	-2.2951545	0.7836589	-0.0007114
C	4.6567956	-1.9609924	-0.6412765	N	2.3853235	-1.7047931	-0.0095844
C	5.9676436	-2.4177914	-0.4478255	C	-1.8856005	-2.3228291	1.3735886
H	6.1485026	-3.4446554	-0.1471385	H	-1.6554275	-1.9099991	2.3595086
C	7.0266376	-1.5348304	-0.6418985	H	-1.4707525	-3.3308111	1.2826206
H	8.0518966	-1.8606044	-0.4937745	H	-2.9646245	-2.3578771	1.2150606
C	6.7500606	-0.2203394	-1.0134005	C	1.5125475	0.1780139	-1.5547924
H	7.5492406	0.5025186	-1.1452085	C	2.2592635	1.2619089	-2.0263374
C	5.4191496	0.1486916	-1.2295615	H	3.3253435	1.1487859	-2.1899684
C	5.0844976	1.5430126	-1.7274305	C	1.6193215	2.4723099	-2.2851324
H	5.9349216	2.2150836	-1.5366065	H	2.1800645	3.3215129	-2.6628044
H	4.9683996	1.4861896	-2.8153815	C	0.2525985	2.5846509	-2.0345684
C	3.4498846	-2.8276414	-0.2993475	H	-0.2717525	3.5198559	-2.2008474
H	2.5938666	-2.4572264	-0.8707645	C	-0.4320375	1.4699839	-1.5507984
H	3.6479656	-3.8600374	-0.6136405	C	-1.9151645	1.5123979	-1.2412404
C	3.4422726	3.2891146	-2.0749235	H	-2.2618605	2.5541939	-1.1920094
H	4.1891476	4.0944416	-2.0159355	H	-2.4547035	1.0315589	-2.0637934
H	2.4664866	3.6402766	-1.7376115	C	2.1403795	-1.1835831	-1.3540954
C	4.0047786	-3.5582314	1.9962005	H	1.4886595	-1.8874751	-1.8995114
H	4.9424206	-3.0118734	2.1946065	H	3.0948845	-1.1760791	-1.9030784
H	3.5194546	-3.7509594	2.9596955	C	-3.7459275	0.4884889	-0.0077254
C	3.1722096	-0.4858184	1.9906535	H	-4.3383785	1.4137649	-0.0005884
C	3.9956746	-0.4231084	3.1228175	H	-3.9991475	-0.1034401	0.8723786
H	3.9806166	-1.2325224	3.8448335	C	2.8048115	-3.0965531	-0.0254234
C	4.8295866	0.6757076	3.3023155	H	3.4282315	-3.2945191	-0.9038464
H	5.4768606	0.7437146	4.1715215	H	1.9607265	-3.8077371	-0.0424594
C	4.8385026	1.6760236	2.3324295	N	0.1736975	0.2615909	1.3638836
H	5.5036946	2.5293886	2.4144895	C	1.4990535	0.1403579	1.5711926
C	3.9696516	1.5689456	1.2452315	C	2.2440945	1.2107219	2.0749076
C	3.9058376	2.6475286	0.1897875	H	3.3080035	1.0904779	2.2473826
H	4.7517866	3.3409596	0.3051945	C	1.6048095	2.4170689	2.3538776
H	2.9657376	3.1942176	0.3270595	H	2.1639375	3.2557989	2.7565256
C	2.3562126	-1.7399144	1.6894385	C	0.2411285	2.5395569	2.0915276
H	1.5584626	-1.4657344	0.9983585	H	-0.2819745	3.4725379	2.2735106
H	1.8941536	-2.0899864	2.6215495	C	-0.4419135	1.4382589	1.5758206
H	3.3674356	2.9522456	-3.1091425	C	-1.9222115	1.4917039	1.2538636
H	4.2711206	-4.5275384	1.5601565	H	-2.2641265	2.5356339	1.2179546
Pd	-2.4414804	-1.0636924	-0.9023445	H	-2.4705375	1.0008369	2.0645746
N	-3.8921084	0.9055256	-1.0156585	C	2.1229015	-1.2189411	1.3448696
N	-4.7436304	-1.9259204	-0.9752195	H	1.4594305	-1.9333931	1.8617966
N	-1.8890134	2.4222746	1.2295565	H	3.0694145	-1.2308801	1.9073876

C	-1.7116604	-2.9591624	-0.5634735	H	-3.9947775	-0.0871841	-0.8999484
H	-0.6249364	-2.9750764	-0.4849695	H	3.4131905	-3.3190181	0.8576056
H	-2.0306584	-3.6310054	-1.3621195	C	-1.8773225	-2.2926271	-1.4335844
H	-2.1555024	-3.2584704	0.3916165	H	-1.8399705	-1.7451091	-2.3793394
C	-3.6083814	2.1669136	-0.6210445	H	-1.2956165	-3.2162751	-1.5153574
C	-4.6080274	3.1461006	-0.5351195	H	-2.9075795	-2.5323601	-1.1683154
H	-4.3357154	4.1601756	-0.2632385				
C	-5.9305274	2.8086806	-0.7924075	13_N ₄ (D)			
H	-6.7186184	3.5527196	-0.7284845	Pd	1.3698914	-0.0004777	0.0000678
C	-6.2249244	1.4868836	-1.1150765	N	-0.3898076	-0.0037677	-1.3793212
H	-7.2474174	1.1699356	-1.2922995	N	0.5481664	-2.3398187	0.0063968
C	-5.1821474	0.5649196	-1.2218345	N	0.5497934	2.3393573	-0.0065172
C	-5.5063244	-0.8542834	-1.6454835	C	2.8876084	0.0117593	1.3944958
H	-6.5898914	-1.0206704	-1.5345985	H	2.4246154	0.1203503	2.3800558
H	-5.2865334	-0.9418564	-2.7156305	H	3.5714994	0.8432033	1.2098958
C	-2.1866264	2.5115696	-0.2055355	H	3.4447114	-0.9271847	1.3472098
H	-1.4671864	1.8987686	-0.7418185	C	-1.0128676	1.1633433	-1.6108602
H	-1.9788394	3.5452456	-0.5009925	C	-2.2838106	1.1981453	-2.1871172
C	-4.9143534	-3.1810284	-1.7337835	H	-2.7721096	2.1478723	-2.3793082
H	-5.9642604	-3.5121874	-1.7381925	C	-2.9147616	-0.0071127	-2.4941492
H	-4.3018874	-3.9662314	-1.2885025	H	-3.9024666	-0.0083937	-2.9443132
C	-2.5128944	3.4286826	2.0718075	C	-2.2826706	-1.2106277	-2.1825932
H	-3.5960194	3.2967046	2.2358885	H	-2.7700206	-2.1615607	-2.3711672
H	-2.0255904	3.4324906	3.0534315	C	-1.0118456	-1.1722747	-1.6063392
N	-3.3968204	-0.6021834	1.2690335	C	-0.2505566	-2.4341927	-1.2396002
C	-2.9648644	0.3170156	2.1597765	H	-0.9463986	-3.2861187	-1.1998062
C	-3.6912064	0.6046756	3.3221685	H	0.4576074	-2.6412867	-2.0494972
H	-3.2904424	1.3098136	4.0422835	C	-0.2529986	2.4279513	-1.2502392
C	-4.9223594	-0.0056634	3.5322695	H	0.4519994	2.6336933	-2.0631882
H	-5.5047174	0.2077576	4.4233705	H	-0.9504586	3.2786023	-1.2112242
C	-5.4044354	-0.8781474	2.5613145	C	1.6068194	-3.3695767	0.0101948
H	-6.3779894	-1.3461664	2.6649735	H	1.1924144	-4.3887057	0.0091358
C	-4.6125764	-1.1583454	1.4455035	H	2.2299484	-3.2440747	0.8972948
C	-5.1126074	-2.1693694	0.4320195	C	1.6092104	3.3683353	-0.0100522
H	-6.2047134	-2.2693554	0.5388895	H	1.1955604	4.3877703	-0.0092272
H	-4.6865054	-3.1430144	0.6995305	H	2.2325544	3.2422953	-0.8969322
C	-1.7014474	1.1050096	1.8385195	N	-0.3901696	0.0039863	1.3788618
H	-1.0771164	0.5128566	1.1724705	C	-1.0113346	1.1729313	1.6060078
H	-1.1467854	1.2603676	2.7728005	C	-2.2820206	1.2121743	2.1825068
H	-4.5928734	-3.0374504	-2.7663585	H	-2.7686666	2.1634483	2.3711808
H	-2.3602944	4.4160406	1.6233915	C	-2.9148916	0.0091013	2.4941768
C	-2.0978544	-1.3623254	-2.9062075	H	-3.9025036	0.0110753	2.9445428
H	-1.3296304	-2.1091774	-3.1078255	C	-2.2848526	-1.1965987	2.1870098
H	-3.0451104	-1.6810764	-3.3489665	H	-2.7737916	-2.1459777	2.3792878
H	-1.7995014	-0.3938084	-3.3135965	C	-1.0139936	-1.1626907	1.6105078
Pd	2.0859496	0.6847456	-1.0625955	C	-0.2550966	-2.4278827	1.2498508
C	1.6618696	0.7254846	-3.1035335	H	-0.9532996	-3.2779087	1.2104808
H	1.0270896	1.5969446	-3.2791135	H	0.4494444	-2.6344027	2.0629998
H	1.1680336	-0.1881154	-3.4390035	C	-0.2492526	2.4343673	1.2392108
H	2.6178226	0.8296216	-3.6253505	H	0.4587504	2.6412613	2.0493008
N	3.1227356	0.5289546	1.1061845	H	-0.9446456	3.2866463	1.1990618
C	-0.1203334	-0.4610194	-0.9810165	H	2.2360764	-3.2438097	-0.8725082
H	0.1954576	-1.2373184	-1.6574805	H	2.2380714	3.2421813	0.8728758
H	0.0531456	-0.6111864	0.0746905	C	2.8880774	-0.0135037	-1.3938052
H	-0.3140654	0.5330656	-1.3547265	H	2.4253734	-0.1219357	-2.3795182
O	0.9474526	2.4951296	-0.5841735	H	3.4455094	0.9252363	-1.3463582
H	0.5877796	2.3879516	0.3101875	H	3.5715904	-0.8452047	-1.2089662
Scheme 6				8_N ₂			
16				Pd	1.8734401	-0.4382271	0.0305879
Pd	-1.1236959	0.0009213	-0.0000001	N	0.0521931	0.0163069	-1.4343021
N	0.4724111	-0.0003877	1.3981029	N	0.0213511	-0.0574581	1.4250799
N	-0.6217479	-2.1439277	0.0000029	N	-1.3290719	-2.7266311	-0.0439481
N	-0.6180279	2.1450573	-0.0000031	N	0.3852391	2.9932159	0.0492639
C	-2.6208129	0.0021233	-1.4313911	C	3.4202381	0.1196399	-1.2104841
H	-2.1438919	0.0002713	-2.4128741	H	3.6666031	1.1222639	-0.8519331
H	-3.2299979	0.8955663	-1.2906491	H	3.0033791	0.1380309	-2.2185261
H	-3.2332959	-0.8887737	-1.2888421	H	4.3024971	-0.5136771	-1.1647591
C	1.0404171	1.1775293	1.6788469	C	3.1828371	-0.5678541	1.6006839

C	2.2570461	1.2153143	2.3581609	H	4.2219091	-0.5984261	1.2759979
H	2.7309131	2.1581963	2.6100259	H	2.9289331	-1.4609211	2.1744329
C	2.8539971	-0.0024477	2.7062099	H	2.9909611	0.3287119	2.1948399
H	3.8001831	-0.0032647	3.2381559	C	-0.1855569	1.3074699	-1.7723571
C	2.2549261	-1.2191777	2.3581919	C	-1.2851599	1.6688019	-2.5560651
H	2.7271501	-2.1628757	2.6100809	H	-1.4234249	2.7086909	-2.8321701
C	1.0383701	-1.1792877	1.6788699	C	-2.1791969	0.6922019	-2.9804821
C	0.2045781	-2.3727497	1.2593519	H	-3.0291399	0.9488099	-3.6052531
H	0.8185451	-3.2694147	1.1230379	C	-1.9590379	-0.6208251	-2.5807641
H	-0.5081739	-2.5890717	2.0617069	H	-2.6364809	-1.4133551	-2.8800651
C	0.2086871	2.3724303	1.2593379	C	-0.8457969	-0.9332401	-1.7937781
H	-0.5036859	2.5899573	2.0617089	C	-0.6742949	-2.3671201	-1.2979881
H	0.8242021	3.2680393	1.1230509	H	-1.0801249	-3.0323281	-2.0697791
C	-1.7481129	-3.1282927	0.0000009	H	0.3853681	-2.5971171	-1.2096991
H	-1.3537619	-4.1506567	-0.0000031	C	-0.6882709	-2.4214701	1.2297359
H	-2.3597699	-2.9830547	-0.8897321	H	0.3800571	-2.6297511	1.1411439
C	-1.7426409	3.1314153	-0.0000011	H	-1.0901499	-3.1234611	1.9704799
H	-1.3464799	4.1530813	0.0000029	C	-0.8724409	-1.0097251	1.7738159
H	-2.3545679	2.9872863	0.8897289	C	-1.9739559	-0.7071431	2.5797819
N	0.4724111	-0.0003917	-1.3981031	H	-2.6567269	-1.4986881	2.8695939
C	1.0404141	1.1775263	-1.6788531	C	-2.1719449	0.6000709	3.0123189
C	2.2570431	1.2153113	-2.3581681	H	-3.0116099	0.8509439	3.6530999
H	2.7309071	2.1581923	-2.6100381	C	-1.2712179	1.5797799	2.6058219
C	2.8539971	-0.0024517	-2.7062101	H	-1.3937329	2.6119789	2.9159189
H	3.8001831	-0.0032697	-3.2381561	C	-0.1871479	1.2265569	1.7978479
C	2.2549291	-1.2191817	-2.3581851	C	0.7581881	2.3094119	1.2801969
H	2.7271561	-2.1628797	-2.6100691	H	0.8546831	3.0721759	2.0633679
C	1.0383741	-1.1792917	-1.6788631	H	1.7588501	1.8829709	1.1363059
C	0.2045851	-2.3727537	-1.2593401	C	0.7336441	2.4016159	-1.2372131
H	0.8185551	-3.2694147	-1.1230181	H	1.7546591	2.0226109	-1.1684911
H	-0.5081639	-2.5890847	-2.0616971	H	0.7488341	3.2153999	-1.9718851
C	0.2086811	2.3724263	-1.2593501	C	-2.7821889	-2.7223541	-0.0475721
H	-0.5036959	2.5899453	-2.0617191	H	-3.2451429	-1.7218681	-0.0245051
H	0.8241921	3.2680383	-1.1230701	H	-3.1470629	-3.2807921	0.8211659
H	-2.3597679	-2.9830627	0.8897359	H	-3.1426269	-3.2382951	-0.9438151
H	-2.3545669	2.9872943	-0.8897321	C	-0.8258619	3.7951679	0.0920749
C	-2.6208129	0.0021363	1.4313909	H	-1.7649429	3.2178909	0.0828199
H	-2.1438909	0.0004263	2.4128749	H	-0.8391229	4.4734109	-0.7674241
H	-3.2300799	0.8955093	1.2905569	H	-0.8188729	4.4119549	0.9971409
H	-3.2332139	-0.8888317	1.2889339	C	2.6941251	-2.2835271	-0.4721011
				H	2.5481231	-2.4072871	-1.5443411
				H	3.7441431	-2.3583581	-0.2052391
				H	2.1000491	-2.9861831	0.1114249
8_N ₃				8_N ₄			
Pd	-1.4477325	-0.9048513	-0.0000146	Pd	-1.4273381	0.6687891	-0.0232533
N	0.2138065	0.1142887	-1.3977436	N	0.4906829	-0.3381399	-1.3441923
N	-2.0242735	1.3488997	0.0000324	N	1.4497689	2.2255371	-0.1146663
N	2.5953825	-1.8016023	-0.0000406	N	-1.7502381	-1.6621849	0.0157397
C	-2.7866075	-1.3807183	1.4771244	C	-2.9056601	0.9135461	1.3705237
H	-3.6823965	-1.8576923	1.0822584	H	-2.6771201	0.1598401	2.1273497
H	-3.0366765	-0.4323453	1.9558214	H	-3.8800451	0.7353151	0.9161417
H	-2.2856865	-2.0368433	2.1889794	H	-2.8690681	1.9075421	1.8114437
C	-1.2132495	-2.9763573	-0.0000536	C	0.2499419	-1.6519659	-1.5410163
H	-2.1889925	-3.4598233	-0.0000456	C	1.2158679	-2.5326059	-2.0282123
H	-0.6699425	-3.2694723	-0.8981186	H	0.9702639	-3.5780979	-2.1822443
C	1.4422355	-0.3458223	-1.7253686	C	2.4930249	-2.0486279	-2.2960603
C	2.3591995	0.4599357	-2.4121766	H	3.2667259	-2.7037979	-2.6837563
H	3.3178505	0.0442627	-2.7027776	C	2.7653579	-0.7177749	-2.0086853
C	2.0376325	1.7798337	-2.7050036	H	3.7625189	-0.3139759	-2.1492593
H	2.7373805	2.4190297	-3.2342426	C	1.7484439	0.1129421	-1.5181433
C	0.8054215	2.2715867	-2.2830946	C	2.1111779	1.5625931	-1.2336953
H	0.5266555	3.3054687	-2.4580316	H	3.2127369	1.6176621	-1.1548083
C	-0.0813235	1.4095777	-1.6374496	H	1.8513279	2.1381461	-2.1316013
C	-1.4504395	1.9217577	-1.2452096	C	-1.1338111	-2.1807739	-1.2325843
H	-1.4273755	3.0191177	-1.1836366	H	-1.8069551	-1.9000799	-2.0502073
H	-2.1469135	1.6728117	-2.0533786	H	-1.1043701	-3.2800219	-1.2123933
C	1.8631745	-1.7361063	-1.2628046	C	1.6470229	3.6759171	-0.2315663
H	0.9832415	-2.3709743	-1.1853366	H	2.7089399	3.9672771	-0.1561043
H	2.5128915	-2.1689813	-2.0327166	H	1.0985639	4.1933171	0.5591807
C	-3.4836495	1.6304927	0.0000174	C	-3.1682601	-2.0989649	0.0347027

H	-3.6753385	2.7119827	0.0000394	H	-3.2424971	-3.1949139	0.0636877
H	-3.9474665	1.1937517	0.8845664	H	-3.6825431	-1.7432039	-0.8584863
C	3.9351945	-1.2398973	-0.0000236	N	0.3679309	-0.1895029	1.3862107
C	3.9815815	-0.1377163	0.0000004	C	0.2074699	-1.5061169	1.6276267
H	4.4758295	-1.5975953	0.8827944	C	1.2017059	-2.2894719	2.2172357
N	0.2138125	0.1142317	1.3977454	H	1.0221729	-3.3430099	2.4044107
C	1.4422415	-0.3458953	1.7253464	C	2.4183309	-1.7005419	2.5428247
C	2.3592115	0.4598317	2.4121804	H	3.2085849	-2.2784679	3.0114397
H	3.3178635	0.0441447	2.7027574	C	2.6153419	-0.3656909	2.2070367
C	2.0376485	1.7797177	2.7050674	H	3.5699669	0.1157971	2.3890667
H	2.7374015	2.4188907	3.2343284	C	1.5799049	0.3624391	1.6106787
C	0.8054345	2.2714907	2.2831874	C	1.8423519	1.8080351	1.2336487
H	0.5266725	3.3053657	2.4581704	H	2.9120839	2.0093981	1.4244757
C	-0.0813155	1.4095107	1.6375104	H	1.2849919	2.4459431	1.9315697
C	-1.4504345	1.9217067	1.2452994	C	-1.1133541	-2.1521649	1.2650777
H	-1.4273685	3.0190697	1.1837744	H	-1.8254811	-1.9561249	2.0741247
H	-2.1468995	1.6727287	2.0534664	H	-0.9838481	-3.2434309	1.2256497
C	1.8631695	-1.7361623	1.2627214	H	1.2660879	4.0288841	-1.1935853
H	0.9832335	-2.3710253	1.1852274	H	-3.6713601	-1.6909079	0.9115097
H	2.5128855	-2.1690703	2.0326144	C	-2.7704611	0.9880281	-1.5313283
H	-3.9474375	1.1937937	-0.8845686	H	-3.1196061	0.0023861	-1.8422953
H	4.4758365	-1.5975563	-0.8828536	H	-3.6138171	1.6102021	-1.2369963
H	-0.6699115	-3.2695003	0.8979834	H	-2.2070481	1.4646251	-2.3356673
C	-2.7866265	-1.3806473	-1.4771596	C	-1.4108231	2.7335771	-0.0209363
H	-3.6824065	-1.8576473	-1.0823046	H	-0.8913951	3.0332461	0.8883877
H	-3.0367105	-0.4322473	-1.9557966	H	-0.8624531	3.0408981	-0.9074093
H	-2.2857165	-2.0367293	-2.1890616	H	-2.4217391	3.1386761	-0.0305883
TS8_N ₂ N ₃ frequency=-311.18 cm ⁻¹				TS8_N ₃ N ₄ frequency=-255.28 cm ⁻¹			
Pd	-1.2403196	-1.2325517	-0.0411721	Pd	1.2226443	-0.9581711	-0.0029253
N	0.1710684	0.0742743	1.3732139	N	-0.2612407	0.3804579	-1.3546543
N	0.2104814	0.1024943	-1.3799581	N	-2.3993737	-1.7154501	0.0077247
N	2.7572094	-1.6696557	-0.0123971	N	2.2027563	1.1746809	-0.0024963
N	-2.2356866	1.8858473	-0.0022701	C	2.4806353	-1.7025231	1.4274057
C	-2.8162626	-1.6034767	1.2173439	H	1.9905623	-1.4609941	2.3736657
H	-3.4944846	-0.7822337	0.9715249	H	3.4325533	-1.1802671	1.3271127
H	-2.4290816	-1.5201927	2.2337809	H	2.6371463	-2.7756661	1.3441127
H	-3.3087966	-2.5605267	1.0622329	C	0.2470843	1.6159359	-1.5410763
C	-2.3658476	-1.9621897	-1.5813471	C	-0.5270677	2.6821059	-2.0011513
H	-3.0464946	-2.7588957	-1.2876651	H	-0.0726107	3.6545029	-2.1590373
H	-1.6643806	-2.3065147	-2.3437241	C	-1.8833757	2.4780289	-2.2361343
H	-2.9302576	-1.0965867	-1.9379021	H	-2.5117217	3.2859439	-2.5975433
C	-0.2654306	1.3401493	1.5813139	C	-2.4195087	1.2219269	-1.9745043
C	0.5719964	2.3322463	2.0942709	H	-3.4769117	1.0280409	-2.1167883
H	0.1828984	3.3327993	2.2471029	C	-1.5865527	0.1891739	-1.5291833
C	1.8852794	2.0146543	2.4302919	C	-2.1688637	-1.1923051	-1.3299453
H	2.5434904	2.7613833	2.8634069	H	-3.1266797	-1.2015461	-1.8731163
C	2.3303964	0.7193333	2.2013389	H	-1.5165467	-1.8874781	-1.8897673
H	3.3437344	0.4273623	2.4538789	C	1.7166823	1.8236999	-1.2494143
C	1.4647234	-0.2249227	1.6344599	H	2.3007783	1.3944959	-2.0710613
C	2.0073954	-1.5946627	1.2427459	H	1.9391563	2.9002739	-1.2305943
H	2.6833354	-1.9365927	2.0346849	C	-3.0949347	-2.9893341	-0.0260763
H	1.1850174	-2.3053577	1.1972389	H	-4.1626477	-2.8852331	-0.2807413
C	2.0252794	-1.5706327	-1.2747381	H	-3.0284687	-3.4838511	0.9464797
H	1.1845764	-2.2673427	-1.2511721	C	3.6844623	1.2317959	-0.0086873
H	2.7035234	-1.9120137	-2.0650581	H	4.0380323	2.2713239	-0.0462553
C	1.5020444	-0.1892447	-1.6446491	H	4.0759503	0.6995719	-0.8765413
C	2.3666974	0.7698373	-2.1871501	N	-0.2424797	0.3689619	1.3651457
H	3.3824494	0.4894873	-2.4432701	C	0.2564243	1.6087179	1.5473547
C	1.9133454	2.0676093	-2.3887551	C	-0.5245687	2.6677149	2.0120307
H	2.5694284	2.8270383	-2.8026041	H	-0.0785887	3.6447169	2.1657047
C	0.5954284	2.3727703	-2.0559131	C	-1.8771877	2.4502419	2.2577197
H	0.2015274	3.3735463	-2.1947831	H	-2.5103547	3.2525759	2.6231447
C	-0.2384356	1.3661383	-1.5669821	C	-2.4034247	1.1883319	2.0030187
C	-1.7089496	1.6504303	-1.3498791	H	-3.4575397	0.9839599	2.1550757
H	-1.9437216	2.5460823	-1.9420541	C	-1.5637597	0.1638029	1.5520097
H	-2.2588886	0.8335453	-1.8458391	C	-2.1285557	-1.2250051	1.3538887
C	-1.7272186	1.6546523	1.3544969	H	-3.0647687	-1.2546201	1.9299337
H	-2.2983056	0.8558083	1.8511079	H	-1.4419617	-1.9154291	1.8724687
H	-1.9434816	2.5631153	1.9333929	C	1.7230353	1.8242369	1.2467437
C	4.0805794	-1.0648277	-0.0001641	H	2.3130753	1.3947379	2.0638567

H	4.0895974	0.0378683	0.0095179	H	1.9408523	2.9017399	1.2267527
H	4.6358624	-1.3972867	-0.8834301	H	-2.6428527	-3.6655171	-0.7657633
H	4.6264394	-1.4129287	0.8828449	H	4.0792563	0.7666829	0.8948407
C	-0.9225266	-3.2415397	0.3772289	C	2.4504823	-1.7311581	-1.4451813
H	-0.6914746	-3.2986637	1.4400329	H	3.0085993	-0.8823261	-1.8450963
H	-1.7827116	-3.8568887	0.1313999	H	3.1329793	-2.4814281	-1.0487543
H	-0.0702296	-3.5040657	-0.2481171	H	1.8114823	-2.1625841	-2.2166393
C	-3.6646666	2.1524853	-0.0184671	C	0.4727393	-2.8865561	0.0035347
H	-3.9235346	2.7769433	-0.8806331	H	-0.0002927	-3.0453791	0.9721397
H	-4.2862836	1.2407553	-0.0714061	H	-0.2503737	-2.9489331	-0.8059353
H	-3.9563326	2.7011353	0.8826479	H	1.2658413	-3.6166241	-0.1467983
TS_RE_8_N ₂ frequency=-410.56 cm ⁻¹				TS_RE_8_N ₃ frequency=-515.51 cm ⁻¹			
Pd	1.7664418	-0.0963596	-0.1606673	Pd	1.2704658	-0.8468820	-0.3082516
N	0.0045888	-0.0014816	-1.4306023	N	-0.1286292	-0.2069330	1.3983664
N	0.0636098	-0.0042836	1.4095997	N	1.9766588	1.5505630	0.2476494
N	-0.6530122	-2.9512176	-0.0096733	N	-2.4836712	-1.8185710	-0.3793096
N	-0.3584562	2.9980284	0.0039307	C	2.3741488	-0.9807750	-2.0160406
C	2.9759658	-0.2189476	-1.8134853	H	2.6339618	-2.0126590	-2.2581706
H	3.1748398	0.7977934	-2.1615413	H	3.2825838	-0.3944480	-1.8546386
H	2.4295568	-0.7749206	-2.5773633	H	1.7703418	-0.5459690	-2.8151396
H	3.9126828	-0.7241746	-1.5730923	C	1.5511318	-3.0897510	-0.0978156
C	3.4851468	0.9015404	0.7927807	H	2.3828398	-3.7157580	-0.4091806
H	4.4467248	0.8206054	0.2974267	H	1.0761858	-3.4841760	0.7956974
H	3.5784208	0.9702784	1.8728857	C	-1.3393762	-0.7618240	1.6317764
H	2.9662928	1.7871014	0.4144987	C	-2.2508482	-0.1680830	2.5131854
C	-0.5034492	1.2016414	-1.7910113	H	-3.1967782	-0.6595000	2.7135294
C	-1.6363312	1.2814114	-2.6047273	C	-1.9373622	1.0453130	3.1138024
H	-2.0065302	2.2557354	-2.9044793	H	-2.6311242	1.5220240	3.7992484
C	-2.2658802	0.1163184	-3.0309573	C	-0.7219782	1.6493940	2.8006604
H	-3.1376162	0.1619484	-3.6763103	H	-0.4544102	2.6127360	3.2215464
C	-1.7559052	-1.1081916	-2.6119653	C	0.1625118	0.9988000	1.9396244
H	-2.2216182	-2.0392246	-2.9160913	C	1.5114138	1.6301850	1.6451224
C	-0.6205282	-1.1456406	-1.7986183	H	1.4964298	2.6735200	1.9994244
C	-0.1019602	-2.4827136	-1.2749703	H	2.2609848	1.1120270	2.2561694
H	-0.3277722	-3.2443006	-2.0314923	C	-1.7349242	-2.0168570	0.8595454
H	0.9872238	-2.4331056	-1.1806473	H	-0.8390152	-2.5910720	0.6282494
C	-0.0778882	-2.4920306	1.2504287	H	-2.3604692	-2.6357700	1.5136394
H	1.0064448	-2.4801956	1.1447767	C	3.4223068	1.8250240	0.1913044
H	-0.3155552	-3.2518736	2.0047217	H	3.6720998	2.8394730	0.5380304
C	-0.5593762	-1.1469376	1.7917797	H	3.7784858	1.7127210	-0.8349106
C	-1.6676722	-1.1208166	2.6439687	C	-3.8430602	-1.3244330	-0.2370756
H	-2.1215102	-2.0561046	2.9536227	H	-3.9269022	-0.2541940	0.0161614
C	-2.1684612	0.0965804	3.0912667	H	-4.3869562	-1.4898150	-1.1732666
H	-3.0191102	0.1349604	3.7647137	N	-0.2813232	0.5418280	-1.2731996
C	-1.5547842	1.2637694	2.6508507	C	-1.4680002	0.0728700	-1.7278666
H	-1.9182002	2.2361734	2.9654607	C	-2.4356122	0.9406010	-2.2425006
C	-0.4481362	1.1891324	1.7996097	H	-3.3595902	0.5349320	-2.6399666
C	0.1609118	2.4835834	1.2669587	C	-2.2083352	2.3137390	-2.2263426
H	-0.0110622	3.2610904	2.0209047	H	-2.9498332	3.0039000	-2.6165576
H	1.2409668	2.3688594	1.1755777	C	-1.0205282	2.7844110	-1.6788196
C	0.1441268	2.4792364	-1.2620783	H	-0.8167332	3.8486080	-1.6156616
H	1.2233028	2.3248534	-1.1720383	C	-0.0715192	1.8695690	-1.2149976
H	-0.0076452	3.2609554	-2.0165253	C	1.2550798	2.4065750	-0.6973366
C	-2.0734632	-3.2581406	0.0015907	H	1.0830398	3.4145440	-0.2856306
H	-2.7389102	-2.3790516	0.0111647	H	1.9067808	2.5434310	-1.5681366
H	-2.3046642	-3.8638316	0.8841077	C	-1.7771742	-1.4141170	-1.5934096
H	-2.3207312	-3.8576536	-0.8810113	H	-0.8452352	-1.9797260	-1.6595136
C	-1.7408222	3.4468914	0.0115337	H	-2.4031632	-1.7107840	-2.4435226
H	-2.4917572	2.6395874	0.0184267	H	3.9601948	1.1096010	0.8195074
H	-1.9238122	4.0686294	-0.8713953	H	-4.3541642	-1.8961130	0.5447144
H	-1.9124762	4.0723634	0.8938387	H	0.8418538	-3.0686920	-0.9285236
C	3.2544618	-1.1512966	1.0524527	C	2.9111278	-1.9056140	0.7474494
H	2.9436648	-2.0104586	0.4504957	H	3.7653918	-2.1003050	0.1055614
H	4.3389738	-1.1288976	1.0469817	H	2.9910598	-0.8946310	1.1641614
H	2.8607468	-1.1972176	2.0643877	H	2.8896348	-2.5889350	1.5916584
TS_RE_8_N ₄ frequency=-509.51 cm ⁻¹				TS_Rot_8_N ₄ frequency=-83.33 cm ⁻¹			
Pd	-1.6277858	0.1169989	-0.1159410	Pd	-1.6386108	0.0347289	-0.0469207
N	0.9369752	-0.3854871	-1.3714920	N	0.2495492	-0.0247671	1.3603463
N	0.7924672	2.4226439	-0.5153790	N	-0.3658018	-2.4443651	-0.2400037
N	-1.1317328	-2.1110511	-0.1337390	N	-0.1750008	2.4761839	-0.1947587

C	-3.2684278	0.8235829	1.2456230	C	-2.8554108	1.4670139	0.7785873
H	-3.0076988	-0.1174631	1.7436490	H	-2.9720318	2.2530269	0.0381493
H	-4.2328758	0.7327299	0.7553630	H	-2.3106518	1.8058499	1.6601123
H	-3.2847268	1.5979239	2.0063150	H	-3.8275398	1.0765369	1.0659963
C	1.0816782	-1.7170311	-1.3265910	C	0.9333572	1.1041719	1.6419803
C	2.3263182	-2.3465201	-1.3945940	C	2.1263172	1.0751459	2.3699573
H	2.3995402	-3.4292211	-1.3701140	H	2.6409452	2.0031249	2.5957923
C	3.4674542	-1.5505231	-1.4859420	C	2.6501382	-0.1474031	2.7762033
H	4.4528592	-2.0015681	-1.5498980	H	3.5685902	-0.1935991	3.3527773
C	3.3213802	-0.1675471	-1.4539640	C	2.0052552	-1.3115691	2.3705313
H	4.1900692	0.4828759	-1.4766180	H	2.4224602	-2.2871841	2.5962033
C	2.0340112	0.3834379	-1.3830850	C	0.8175272	-1.2166151	1.6419083
C	1.8684032	1.8937789	-1.3604140	C	0.1502412	-2.4857281	1.1461793
H	2.8451822	2.3475199	-1.1102590	H	0.8575932	-3.3206331	1.2781913
H	1.6425862	2.2110529	-2.3858570	H	-0.7059638	-2.7043761	1.7940733
C	-0.1875888	-2.5332121	-1.2128940	C	0.4019702	2.4456539	1.1641713
H	-0.7472718	-2.4530481	-2.1506560	H	-0.3888998	2.7647449	1.8520763
H	0.0679802	-3.5938181	-1.0762320	H	1.2103302	3.1881169	1.2680973
C	0.5343552	3.8203979	-0.8877280	C	-1.1834048	-3.6560221	-0.4632877
H	1.4078642	4.4762399	-0.7270740	H	-0.5648338	-4.5670151	-0.4724667
H	-0.2955578	4.2184539	-0.2984470	H	-1.6979158	-3.5830891	-1.4250347
C	-2.3471658	-2.9566451	-0.2592160	C	-0.9179718	3.7417109	-0.3619167
H	-2.1083068	-4.0145621	-0.0837710	H	-0.2459398	4.6144529	-0.3536067
H	-2.7642848	-2.8558921	-1.2609480	H	-1.6427538	3.8707699	0.4418283
N	0.1932652	0.0308839	1.2794180	N	0.8488542	-0.0156781	-1.3594217
C	0.3975082	-1.2380551	1.6918320	C	1.5633102	1.1164529	-1.4370067
C	1.4736942	-1.5956461	2.5042990	C	2.9400182	1.1193559	-1.6816977
H	1.5938912	-2.6247111	2.8261110	H	3.4786372	2.0589559	-1.7505357
C	2.3889242	-0.6156291	2.8743870	C	3.6007172	-0.0976561	-1.8247407
H	3.2296222	-0.8557691	3.5175040	H	4.6676862	-0.1296431	-2.0221487
C	2.2360222	0.6648849	2.3531410	C	2.8702702	-1.2725391	-1.6722687
H	2.9693282	1.4369199	2.5595700	H	3.3533342	-2.2423871	-1.7342847
C	1.1409102	0.9598159	1.5342790	C	1.4953852	-1.1874631	-1.4297017
C	1.0362152	2.3506459	0.9303500	C	0.6793592	-2.4511211	-1.2844897
H	1.9530062	2.8994789	1.2131710	H	1.3641422	-3.3034521	-1.1412747
H	0.2089342	2.8771349	1.4203910	H	0.1625402	-2.6273621	-2.2354967
C	-0.5945138	-2.2928601	1.2472790	C	0.8204572	2.4228189	-1.2837467
H	-1.4585948	-2.2680901	1.9211300	H	0.2720542	2.6137189	-2.2140767
H	-0.1427128	-3.2895471	1.3518630	H	1.5539942	3.2400309	-1.1810967
H	0.2581332	3.8746489	-1.9442030	H	-1.9273308	-3.7695331	0.3252363
H	-3.0961128	-2.6370111	0.4672750	H	-1.4515648	3.7323039	-1.3159827
C	-3.0435538	-0.1269251	-1.5558690	C	-3.0447358	-1.2693861	0.6883013
H	-2.5269808	-0.6210101	-2.3843190	H	-2.6782768	-1.5400481	1.6805643
H	-3.8569728	-0.7486451	-1.1754580	H	-4.0359008	-0.8302871	0.7573853
H	-3.4344758	0.8361019	-1.8879240	H	-3.0645108	-2.1144381	0.0083713
C	-2.3522458	2.1731569	0.0700460	C	-2.8723008	0.1291939	-1.6630257
H	-1.9229208	2.7782729	0.8613240	H	-2.4671888	0.9560469	-2.2522907
H	-1.6854738	2.2018109	-0.8042290	H	-2.7505878	-0.8199371	-2.1903177
H	-3.3305978	2.5360939	-0.2314650	H	-3.9199058	0.3031849	-1.4214217
Scheme 8				TS_RE_13(Me-Me) frequency=-526.91 cm ⁻¹			
TS_RE_1(Me-Me) frequency=-549.38 cm ⁻¹				Pd 1.4032968 -0.0001406 -0.0002948			
Pd	2.2029080	0.0008837	0.0009369	N	-0.4781652	0.0160704	-1.3945578
N	0.1378230	-0.0236973	-1.4148331	N	0.4997068	-2.3114686	-0.0173628
N	0.1343680	0.0239747	1.4157419	N	0.5003408	2.3112504	0.0177402
N	-0.2668280	-3.0143843	0.0510239	C	3.4236328	-0.1009126	0.9811792
N	-0.2693360	3.0143107	-0.0509981	H	2.7959788	0.2051514	1.8301832
C	4.1899500	-0.2294203	-0.9070551	H	4.2999368	0.5428024	0.9993072
H	4.4888010	0.6752637	-1.4371551	C	3.7236938	-1.1389176	1.1106022
H	3.5072350	-0.8136543	-1.5572841	C	-1.1155652	1.1802024	-1.5677278
H	5.0637360	-0.8668943	-0.7639311	C	-2.4205052	1.2229714	-2.0636418
C	4.1874120	0.2322387	0.9135149	H	-2.9237972	2.1727614	-2.2135678
H	4.4860530	-0.6721733	1.4442059	C	-3.0647022	0.0177534	-2.3470088
H	3.5023650	0.8155257	1.5622419	H	-4.0775882	0.0185224	-2.7373998
H	5.0607560	0.8708217	0.7726949	C	-2.4134572	-1.1891346	-2.0867538
C	-0.4448900	1.1361027	-1.7684811	H	-2.9113982	-2.1386336	-2.2551588
C	-1.6281380	1.1635847	-2.5170621	C	-1.1089622	-1.1487056	-1.5899978
H	-2.0580700	2.1146937	-2.8159081	C	-0.3096552	-2.3984366	-1.2645548
C	-2.2300410	-0.0384063	-2.8808421	H	-0.9785412	-3.2720926	-1.2320048
H	-3.1417150	-0.0445043	-3.4719341	H	0.3971418	-2.5690326	-2.0841428
C	-1.6401340	-1.2324973	-2.4738311	C	-0.3224492	2.4272094	-1.2178278

H	-2.0794150	-2.1895573	-2.7383331	H	0.3736368	2.6255844	-2.0403798
C	-0.4554680	-1.1902183	-1.7284131	H	-0.9974252	3.2945214	-1.1547358
C	0.2065200	-2.4678553	-1.2211011	C	1.5233778	-3.3776286	-0.0247978
H	0.0685870	-3.2535283	-1.9767721	H	1.0759648	-4.3829696	-0.0412838
H	1.2785000	-2.2662133	-1.1196341	H	2.1464368	-3.2892396	0.8673932
C	0.2235020	-2.4222513	1.2964239	C	1.5242898	3.3771474	0.0252462
H	1.2920860	-2.2086333	1.1710059	H	1.0771288	4.3825954	0.0419152
H	0.1077860	-3.1838473	2.0800459	H	2.1472608	3.2887314	-0.8670028
C	-0.4480440	-1.1363103	1.7681419	N	-0.4781992	-0.0160216	1.3952502
C	-1.6329230	-1.1648493	2.5141189	C	-1.1088192	1.1489084	1.5902072
H	-2.0626930	-2.1163123	2.8120799	C	-2.4136362	1.1897324	2.0860992
C	-2.2366700	0.0366397	2.8765149	H	-2.9114362	2.1393694	2.2541512
H	-3.1496590	0.0419497	3.4655849	C	-3.0653762	-0.0169816	2.3459532
C	-1.6469090	1.2312587	2.4708289	H	-4.0785152	-0.0174696	2.7356902
H	-2.0876070	2.1879267	2.7343979	C	-2.4213392	-1.2223836	2.0629782
C	-0.4605470	1.1899697	1.7280349	H	-2.9250092	-2.1720316	2.2125452
C	0.2015670	2.4681567	1.2221979	C	-1.1160552	-1.1799526	1.5679272
H	0.0612780	3.2537277	1.9775429	C	-0.3230502	-2.4271066	1.2182792
H	1.2739340	2.2674377	1.1231629	H	-0.9980892	-3.2943816	1.1553602
C	0.2243750	2.4226587	-1.2952821	H	0.3730668	-2.6253646	2.0408272
H	1.2928820	2.2100187	-1.1674771	C	-0.3089402	2.3983444	1.2650152
H	0.1097020	3.1841327	-2.0791741	H	0.3979868	2.5684544	2.0845862
C	-1.6414410	-3.4734743	0.0673749	H	-0.9774042	3.2723244	1.2326132
H	-2.4034850	-2.6746273	0.0549369	H	2.1596248	-3.2641806	-0.9047238
H	-1.8110140	-4.0792933	0.9657229	H	2.1605658	3.2634084	0.9051132
H	-1.8196670	-4.1152903	-0.8039191	C	3.4239858	0.1002974	-0.9812338
C	-1.6443090	3.4721977	-0.0704831	H	2.7967648	-0.2063036	-1.8303518
H	-2.4056820	2.6726857	-0.0598551	H	3.7236748	1.1383964	-1.1107888
H	-1.8123490	4.0779497	-0.9691661	H	4.3005868	-0.5430216	-0.9988638
H	-1.8250900	4.1137847	0.8004509				
TS_RE_7(Me-Me) frequency=-466.45 cm ⁻¹				TS_RE_7(Me-OH) frequency=-500.85 cm ⁻¹			
Pd	1.6876309	-0.8531681	0.0049719	Pd	-1.6401387	-0.6761864	-0.3777108
N	-0.0784941	-0.4406181	1.2503429	N	0.3927013	0.7379216	-1.3293488
N	1.9237269	1.2984429	0.2849459	N	-1.9377207	1.3684886	0.3311822
N	-2.4691651	-2.0353091	-0.5955481	N	2.3516753	-1.9403274	-0.8447388
C	3.0178399	-1.0470771	-1.7327961	C	-2.8865547	-2.4289124	0.6181602
H	3.6174539	-0.1746611	-1.9761251	H	-3.4043427	-1.5748364	1.0570282
H	2.0315969	-0.9584801	-2.2082421	H	-2.2659317	-2.9676104	1.3219382
H	3.4857089	-1.9608901	-2.0871331	H	-3.5641687	-3.0542884	0.0490632
C	-1.2165481	-1.1590261	1.4147359	C	1.6207733	0.3336576	-1.6900478
C	-2.1566311	-0.7635871	2.3774229	C	2.6905623	1.2398236	-1.7488158
H	-3.0290201	-1.3860051	2.5402239	H	3.6655583	0.9076986	-2.0896638
H	-1.9797681	0.4105759	3.0978999	C	2.4843573	2.5617216	-1.3649388
C	-2.7071271	0.7211229	3.8413719	H	3.2978673	3.2797976	-1.4006268
C	-0.8628711	1.1977109	2.8263559	C	1.2198563	2.9499606	-0.9181988
H	-0.7067571	2.1462079	3.3291889	H	1.0316113	3.9661626	-0.5862418
C	0.0691039	0.7350239	1.9031119	C	0.1985953	1.9995196	-0.9241958
C	1.3287259	1.5235429	1.6406369	C	-1.2171947	2.3668386	-0.5296048
H	1.1478229	2.5950169	1.7976299	H	-1.2298437	3.3429626	-0.0268658
H	2.0881999	1.2190839	2.3693779	H	-1.8161497	2.4650636	-1.4405748
C	-1.5363861	-2.3339431	0.4895969	C	1.8090573	-1.1572504	-1.9550628
H	-0.6042191	-2.7209201	0.0775579	H	0.8417963	-1.5835614	-2.2334738
H	-1.9898411	-3.1236421	1.1006509	H	2.4913473	-1.2858014	-2.8044528
C	3.3400249	1.7608979	0.3372229	C	-3.3705307	1.7760136	0.3811182
H	3.3851879	2.8278809	0.5877109	H	-3.4747047	2.7637236	0.8480152
H	3.8129149	1.6141209	-0.6337231	H	-3.9384877	1.0475156	0.9619772
C	-3.8431201	-1.7403271	-0.2328391	C	3.7356523	-1.6804534	-0.4918818
H	-4.0109421	-0.7396101	0.2022179	H	3.9141653	-0.7321494	0.0441352
H	-4.4772211	-1.8254641	-1.1220921	H	4.1083663	-2.4960144	0.1376492
N	-0.4496311	0.4859559	-1.4125251	N	0.0148693	-0.5434004	1.1702432
C	-1.7092361	0.1121829	-1.6787281	C	1.1542853	-1.2637854	1.2773002
C	-2.7500011	1.0526319	-1.7511531	C	2.0905253	-0.9621224	2.2767472
H	-3.7517661	0.7358779	-2.0219531	H	2.9707383	-1.5864014	2.3833032
C	-2.4773031	2.3880819	-1.4735861	C	1.8932903	0.1334386	3.1089802
H	-3.2637471	3.1348539	-1.5240161	H	2.6143473	0.3788106	3.8824462
C	-1.1774321	2.7540379	-1.1150731	C	0.7643123	0.9282866	2.9158172
H	-0.9363361	3.7831239	-0.8677321	H	0.5939473	1.8161136	3.5155962
C	-0.1928781	1.7653679	-1.1050351	C	-0.1551997	0.5521046	1.9402982
C	1.2497649	2.1046709	-0.7993591	C	-1.4296497	1.3393176	1.7413122
H	1.3353109	3.1663039	-0.5338771	H	-1.3056677	2.3652246	2.1122402

H	1.8478509	1.9434349	-1.7014851	H	-2.2192497	0.8775566	2.3445692
C	-1.9644651	-1.3860081	-1.8032221	C	1.4589373	-2.3444504	0.2408712
H	-1.0260351	-1.8710371	-2.0867731	H	0.5284293	-2.7098104	-0.1939478
H	-2.6945711	-1.5679581	-2.6013041	H	1.9413363	-3.1827364	0.7583202
H	3.8878949	1.1980039	1.0925469	H	-3.7780817	1.8179466	-0.6279668
H	-4.1929101	-2.4826201	0.4931769	H	4.3426533	-1.6655504	-1.4036358
C	3.8321699	-1.4686651	0.0824469	C	-3.0678727	-0.5174734	-1.8330188
H	4.7315259	-0.9899491	-0.2911091	H	-4.0684247	-0.4835574	-1.3937218
H	3.6653139	-1.1668351	1.1219639	H	-2.8583877	0.4030906	-2.3842148
H	3.8474509	-2.5501441	0.0199209	H	-3.0047707	-1.3561294	-2.5328638
O	1.3970729	-2.8029351	-0.0111661	O	-1.5190427	-2.6654944	-0.7592308
H	1.5241289	-3.1252771	-0.9166351	H	-2.0694977	-2.8604544	-1.5332648
TS_Rot_RE_7(Me-Me) frequency=-507.69 cm ⁻¹				O ₂ +3MeOH_b3lypD3 Triplet			
Pd	-1.6942562	-0.5665439	-0.4027847	O	0.6669969	1.6367561	0.8646183
N	0.3735958	0.9046931	-1.3131267	O	1.0463049	1.9546671	-0.2478847
N	-1.9786962	1.5185511	0.3410943	H	-2.5052811	1.5669182	-0.5006827
N	2.3028858	-1.7988959	-0.9100757	O	-3.0785531	0.8564611	-0.8240477
C	-2.9907112	-2.2049779	0.4378093	O	-0.1359301	-0.9390059	0.7774393
H	-2.7649372	-1.7256599	1.3933923	H	0.0248159	-0.0017979	0.9777132
H	-2.9534532	-3.2791129	0.5864073	O	3.0577319	0.2744121	-0.9626168
H	-3.9367572	-1.8787439	0.0168803	H	2.4414859	1.0175332	-0.8594017
C	1.6171428	0.5307791	-1.6560427	C	-3.4426881	0.0668631	0.3102793
C	2.6803288	1.4448991	-1.6527497	H	-4.0531061	-0.7634989	-0.0575837
H	3.6677828	1.1307251	-1.9746427	H	-2.5674701	-0.3505889	0.8254083
C	2.4497078	2.7532331	-1.2377757	H	-4.0428651	0.6360541	1.0357593
H	3.2561808	3.4799641	-1.2272867	C	-0.1776821	-1.0563549	-0.6490407
C	1.1665498	3.1148091	-0.8265047	H	-0.3792381	-2.1072088	-0.8776357
H	0.9531998	4.1210931	-0.4801107	H	-0.9794661	-0.4488289	-1.0882837
C	0.1536598	2.1562481	-0.8851527	H	0.7813059	-0.7852549	-1.1107407
C	-1.2750052	2.5062501	-0.5251387	C	3.2787119	-0.2668939	0.3393393
H	-1.3112902	3.4979611	-0.0534037	H	3.9959279	-1.0862609	0.2321263
H	-1.8610712	2.5560641	-1.4481117	H	3.7076689	0.4726841	1.0313583
C	1.8332618	-0.9393019	-1.9965137	H	2.3613299	-0.6766558	0.7838772
H	0.8930558	-1.3470549	-2.3779597				
H	2.5727468	-1.0127809	-2.8027957				
C	-3.4278062	1.8570591	0.3385393				
H	-3.5867202	2.8853141	0.6884363				
H	-3.9621492	1.1674061	0.9938523				
C	3.6699308	-1.5827949	-0.4678647				
H	3.8287778	-0.6693479	0.1296023				
H	3.9975788	-2.4392389	0.1313613				
N	-0.1179882	-0.4979779	1.0914133				
C	0.9977868	-1.2624119	1.1924593				
C	1.8964838	-1.0724529	2.2486873				
H	2.7487418	-1.7363979	2.3395563				
C	1.7052368	-0.0356809	3.1536043				
H	2.3973298	0.1208311	3.9749083				
C	0.6245758	0.8200651	2.9617413				
H	0.4652028	1.6760171	3.6087203				
C	-0.2698202	0.5621191	1.9256163				
C	-1.4745812	1.4566751	1.7375263				
H	-1.2516092	2.4625791	2.1188333				
H	-2.2918332	1.0647781	2.3530873				
C	1.3511298	-2.2622779	0.0931123				
H	0.4471198	-2.5797279	-0.4189237				
H	1.7872628	-3.1472419	0.5719763				
H	-3.8081972	1.7295121	-0.6742827				
H	4.3241608	-1.5255069	-1.3440757				
O	-3.1567112	-0.1924899	-1.6570947				
H	-2.9112742	-0.5443529	-2.5258247				
C	-1.8496092	-2.6345739	-1.1883167				
H	-1.2047832	-2.1630549	-1.9453307				
H	-1.3198062	-3.4731009	-0.7485647				
H	-2.7623492	-2.9459259	-1.6881617				
2_N ₂ _(MeOH) ₃ singlet				2_N ₃ _(MeOH) ₃ singlet			
Pd	0.0252716	-1.5389101	-0.1141691	Pd	0.3326207	-1.4813422	0.0582175
N	-1.1892974	0.0691809	-1.3138481	N	1.2781087	0.3028528	1.2733525
N	-3.6656894	-2.0492961	-0.3425271	N	2.4826457	-2.1117392	0.2264035
N	0.4594096	2.3838899	0.5333849	N	-0.5994123	2.5352818	-0.4595255
C	0.5809016	-3.1716541	0.9850069	C	-0.1481443	-3.1056182	-1.0837525

H	0.0858436	-4.0666531	0.5956819	H	0.0267477	-4.0434382	-0.5528205
H	0.2339526	-2.9434221	1.9976699	H	0.5170487	-3.0230392	-1.9498345
H	1.6646176	-3.2763711	0.9683079	H	-1.1889003	-2.9842662	-1.3751085
C	-0.8331144	1.3683259	-1.4153851	C	0.8257907	1.5667948	1.4074985
C	-1.6783334	2.3075939	-2.0160851	C	1.6323327	2.5636738	1.9708435
H	-1.3504994	3.3375079	-2.1043641	H	1.2276037	3.5600818	2.1082855
C	-2.9205844	1.9056419	-2.4963411	C	2.9431857	2.2666348	2.3300525
H	-3.5873434	2.6181319	-2.9726861	H	3.5874557	3.0309838	2.7538775
C	-3.2906934	0.5714439	-2.3550401	C	3.4217997	0.9756068	2.1187185
H	-4.2503814	0.2156439	-2.7135411	H	4.4459227	0.7081288	2.3559725
C	-2.4081854	-0.3271081	-1.7481391	C	2.5551907	0.0150568	1.5981825
C	-2.8434744	-1.7726001	-1.5244541	C	3.0187347	-1.4124602	1.4294715
H	-3.4267094	-2.0826621	-2.3994051	H	4.1150497	-1.4536672	1.4258015
H	-1.9608234	-2.4202841	-1.4783271	H	2.6724017	-1.9824292	2.2979305
C	0.4951426	1.8136839	-0.8297841	C	-0.5557953	1.9035918	0.8771615
H	1.2013706	0.9854029	-0.8179061	H	-1.1630523	1.0009868	0.8228305
H	0.9006516	2.5957489	-1.4796391	H	-1.0230973	2.6101858	1.5706915
C	-4.9575544	-1.3785151	-0.3229171	C	2.7271037	-3.5663112	0.3982585
H	-4.9051944	-0.2910511	-0.1501601	H	3.8042287	-3.7607142	0.4835435
H	-5.5772084	-1.8124051	0.4692269	H	2.3358177	-4.1075412	-0.4622155
C	-0.3373264	3.6041279	0.6514599	C	0.0457537	3.8446358	-0.5342785
H	-1.4211484	3.4426499	0.5593799	H	1.1423177	3.8126668	-0.4587385
H	-0.1434334	4.0646049	1.6252139	H	-0.2154493	4.3165458	-1.4867055
N	-1.3537304	-0.3603771	1.4558439	N	1.4440747	0.0023188	-1.4730865
C	-1.0454684	0.8654969	1.9424179	C	1.0508687	1.2265838	-1.8872945
C	-1.9765844	1.6146519	2.6714499	C	1.9595297	2.1072478	-2.4912105
H	-1.6839064	2.5805889	3.0681079	H	1.6064357	3.0654028	-2.8559495
C	-3.2539704	1.1093049	2.8876359	C	3.2998857	1.7527938	-2.5992845
H	-3.9854074	1.6727919	3.4592149	H	4.0178327	2.4307668	-3.0508345
C	-3.5720164	-0.1351431	2.3547459	C	3.7080077	0.5191288	-2.0968945
H	-4.5562884	-0.5689011	2.4933789	H	4.7480947	0.2126468	-2.1283435
C	-2.6072354	-0.8429821	1.6303919	C	2.7487997	-0.3315792	-1.5493835
C	-3.0039384	-2.1548231	0.9631589	C	3.1450627	-1.6967742	-1.0452205
H	-3.6987234	-2.6763011	1.6311049	H	4.2340577	-1.7534382	-0.9272835
H	-2.1219904	-2.7917471	0.8451639	H	2.8561147	-2.4357832	-1.7988665
C	0.3315656	1.4572609	1.6799489	C	-0.3823363	1.6659688	-1.6397415
H	1.0729236	0.6674519	1.5770629	H	-1.0414503	0.7946908	-1.5676525
H	0.6058136	2.0445809	2.5634909	H	-0.7023803	2.2575688	-2.5056115
H	-5.4630164	-1.5390261	-1.2814131	H	2.2331877	-3.9211332	1.3020595
H	-0.0322284	4.3075349	-0.1296441	H	-0.3309933	4.4756318	0.2773545
C	0.8327886	-2.5083251	-1.7206801	C	-0.3444983	-2.5434202	1.6676355
H	0.1721726	-3.3381661	-1.9884121	H	0.3376687	-3.3617702	1.9013445
H	0.8651146	-1.7633781	-2.5215511	H	-0.3672653	-1.8093112	2.4782755
H	1.8340936	-2.8660091	-1.4863281	H	-1.3457803	-2.9124772	1.4536705
O	1.9455836	-0.8062861	0.1723889	O	-1.5773923	-0.8405222	-0.0788165
O	2.4629966	-0.8923201	1.4027499	O	-2.1018623	-0.8316212	-1.3815595
H	2.2059516	2.9497159	0.6689299	H	-2.3705993	2.9427398	-0.5671475
O	3.1425446	3.2608429	0.6842899	O	-3.3248463	3.1997398	-0.5728925
O	4.1352836	-0.0421881	-1.2805901	O	-3.8380063	-0.2763382	1.2637285
H	3.3230196	-0.4488051	-0.9247221	H	-2.9935153	-0.5659942	0.8511585
O	4.2554276	-2.9048281	1.2272199	O	-3.7087203	-2.8629402	-1.4190265
H	3.5895406	-2.1728071	1.2744739	H	-3.0831233	-2.0631072	-1.3791635
C	3.5429096	3.4547679	-0.6627181	C	-3.7368583	3.3151528	0.7789695
H	2.9469576	4.2290019	-1.1745691	H	-4.8069243	3.5563298	0.7884865
H	4.5858926	3.7938629	-0.6610881	H	-3.6025003	2.3829408	1.3473265
H	3.4951666	2.5328319	-1.2606491	H	-3.2130363	4.1244568	1.3156605
C	4.9162566	0.3405469	-0.1493331	C	-4.7083273	0.0612008	0.1887215
H	5.8268896	0.8191569	-0.5270871	H	-5.6578153	0.4003838	0.6220465
H	4.3909576	1.0608029	0.4906409	H	-4.3070033	0.8749288	-0.4293015
H	5.2088866	-0.5245561	0.4615549	H	-4.9122603	-0.7988412	-0.4639825
C	4.3989736	-3.2995131	-0.1253351	C	-3.7710253	-3.4484542	-0.1390365
H	4.5071706	-2.4477741	-0.8108521	H	-4.5980403	-4.1735052	-0.1174125
H	5.3042936	-3.9143751	-0.2114701	H	-2.8548143	-4.0079022	0.1239235
H	3.5551646	-3.9152051	-0.4795351	H	-3.9522563	-2.7148522	0.6605195
2_N ₃ -(MeOH) ₃ triplet							
Pd	0.6235661	-1.5265285	-0.1916388				
N	1.2175731	0.1502815	1.2911642				
N	2.9594991	-1.9331495	0.2343712				
N	-0.8020859	2.1721295	-0.5209678				
C	0.4460611	-2.9855575	-1.6284828				

H	0.5233041	-3.9976225	-1.2202998
H	1.2579811	-2.8205155	-2.3471648
H	-0.5230329	-2.8466275	-2.1150788
C	0.5638311	1.3204585	1.4498012
C	1.1411671	2.3837095	2.1539872
H	0.5754591	3.2974445	2.2981062
C	2.4376241	2.2588385	2.6427042
H	2.9082781	3.0770095	3.1792472
C	3.1287951	1.0715655	2.4132062
H	4.1517311	0.9422055	2.7504192
C	2.4857211	0.0320475	1.7408012
C	3.1931081	-1.2924505	1.5441102
H	4.2687371	-1.1635795	1.7315662
H	2.8109241	-1.9832455	2.3038732
C	-0.7933269	1.4884995	0.7906312
H	-1.2739659	0.5194645	0.6746762
H	-1.4233959	2.0916845	1.4527292
C	3.3123821	-3.3614265	0.2990602
H	4.3903821	-3.5031825	0.4682642
H	3.0332741	-3.8447205	-0.6388018
C	-0.3400219	3.5600315	-0.4796188
H	0.7400661	3.6676185	-0.3074298
H	-0.5842319	4.0449425	-1.4299508
N	1.7154591	0.0955785	-1.4303988
C	1.1511721	1.2440155	-1.8629718
C	1.9303131	2.2844795	-2.3812228
H	1.4438551	3.1757865	-2.7614068
C	3.3169081	2.1678695	-2.3822948
H	3.9397861	2.9700395	-2.7663088
C	3.8915911	1.0126085	-1.8595328
H	4.9687161	0.8934255	-1.8085348
C	3.0606211	-0.0098485	-1.3991308
C	3.6688701	-1.3015965	-0.8957078
H	4.7267011	-1.1348185	-0.6476478
H	3.6433971	-2.0189415	-1.7230308
C	-0.3495899	1.4148035	-1.7096778
H	-0.8338099	0.4403145	-1.6960528
H	-0.7241299	1.9662765	-2.5792958
H	2.7659261	-3.8385095	1.1137072
H	-0.8655549	4.0870065	0.3220892
C	-0.1311009	-2.8950285	1.1476272
H	0.6128811	-3.6601275	1.3889742
H	-0.3830279	-2.3282355	2.0516922
H	-1.0325359	-3.3679915	0.7508482
O	-1.8189469	-1.3142075	-0.5099098
O	-2.3777459	-1.2753625	-1.6965648
H	-2.5833039	2.4040595	-0.8017878
O	-3.5470219	2.6032745	-0.8920348
O	-3.2125249	-0.8179605	1.7804442
H	-2.7552939	-1.1355575	0.9737962
O	-4.8866149	-2.2315065	-1.0660978
H	-4.0513379	-1.7800095	-1.3182438
C	-3.8732859	3.5434865	0.1157302
H	-4.9536869	3.7266335	0.0759522
H	-3.6376699	3.1866625	1.1310242
H	-3.3676619	4.5126565	-0.0253258
C	-4.2845599	-0.0005115	1.3194022
H	-4.6978299	0.5363395	2.1814662
H	-3.9582219	0.7410335	0.5766982
H	-5.0875979	-0.5947805	0.8604182
C	-4.5239069	-3.2997315	-0.2075318
H	-5.4212939	-3.8999105	-0.0132768
H	-3.7721019	-3.9697965	-0.6558138
H	-4.1352479	-2.9512435	0.7606462